



ADVANCED LIGHT SOURCE

Five-Year Strategic Plan

FY2022



BERKELEY LAB



U.S. DEPARTMENT OF
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1 Introduction

The Advanced Light Source (ALS) is an electron storage ring–based synchrotron radiation facility that is supported by the Department of Energy’s Basic Energy Sciences program (DOE-BES). The ALS started operation in 1993 and since then has been upgraded continuously to remain one of the brightest soft x-ray sources in the world. The ALS is optimized for x-ray spectroscopy, microscopy, and scattering using intense beams from soft x-ray undulator sources but also serves a broader community conducting research using hard x-rays, infrared (IR), and vacuum ultraviolet (VUV) radiation from superconducting magnets, conventional dipole magnets, and insertion devices. The 1.9 GeV ring hosts world-class endstations and instrumentation at more than 40 beamlines and serves nearly 2000 users who publish more than 900 publications per year and conduct basic, applied, and industrial research in energy science, earth and environmental science, materials science, biology, chemistry, and physics. Our mission is to advance science for the benefit of society by providing our world-class synchrotron light source capabilities and expertise to a broad scientific community. Growing, maintaining, and supporting a vibrant and diverse user community is critical for the ALS’s success as a user facility. To engage the community, ALS scientists reach out through many channels, via attendance at conferences, the organization of workshops, and participation on boards and review committees.

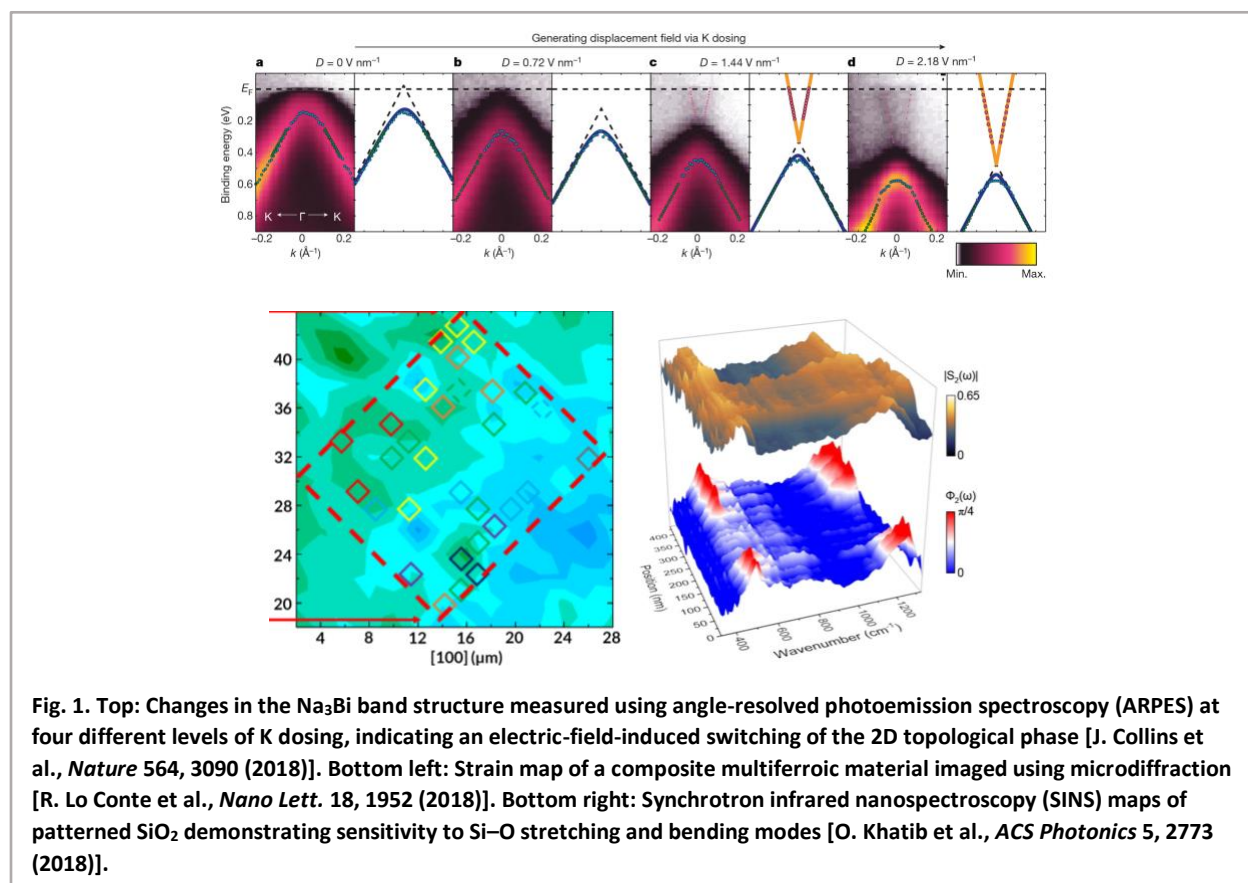
The ALS is the primary BES-funded soft x-ray facility in the U.S., and our ambition is to provide the US and the international community with world-leading x-ray capabilities that enable consequential scientific discoveries and lead to a detailed understanding of laws governing natural processes and the properties of engineered systems. ALS long-term scientific planning is guided by BES Advisory Committee (BESAC) reports on Grand Challenges (2007) and Transformational Opportunities (2015), and investment in new programs is informed by BES reports, for example on quantum materials, electrical storage, and catalysis science, among many others. The ALS participates in Lawrence Berkeley National Laboratory (LBNL) initiatives, for example “Beyond Moore’s Law” and the “Water-Energy Nexus,” and our staff works closely together with other US user facilities and the LBNL Energy Sciences Area to identify new opportunities in x-ray science. The ALS Upgrade Project (ALS-U) is our largest upgrade project since the ALS started operation and will provide the ALS near-diffraction-limited performance in the soft to tender x-ray range, resulting in an increase in brightness and coherent flux of at least two orders of magnitude. Methods based on nanofocusing, diffractive imaging, and coherent scattering will benefit tremendously from the improved performance of the storage ring, and this strategic plan identifies multiple areas where investments into beamline and endstation infrastructure will create opportunities for new scientific discoveries. The ALS-U Project is well underway and reached the Critical Decision-2 (CD-2) milestone in 2021. As part of the strategic planning process, the ALS has identified six Thrust Areas (TAs) centered around cross-cutting themes. These themes guide our long-term strategic planning, as discussed in chapter 2. The chapter also discusses ALS strategic priorities in the areas of accelerator development; the user program; safety; and inclusion, diversity, equity, and accountability (IDEA). A comprehensive list of current accelerator, beamline, detector, optical metrology, and computing projects can be found in chapter 3. New beamline and endstation initiatives are discussed in chapter 4.

2 Strategic priorities

2.1 Thrust Areas

Six TAs have been formed around critical growth areas in x-ray science and instrumentation. The TAs are organized around cross-cutting themes and include scientists from the ALS and closely tied LBNL divisions. Members of the TAs collaboratively develop the science and instrumentation strategy for their area, propose new research and development (R&D) activities to advance these strategies, lead ALS responses to funding opportunities, and reach out to the user community to launch initiatives that result in new beamline projects.

2.1.1 Quantum Materials Research and Discovery



The discovery, synthesis, and characterization of novel functional quantum materials is the central theme of this TA. Soft x-ray spectroscopy, scattering, and microscopy tools have played a major role in the discovery and understanding of the exotic and fascinating physics of many new classes of spin, quantum, and topological materials over the past few decades: oxide and pnictide superconductors, manganites exhibiting colossal magnetoresistance, graphene and other 2D materials, topological insulators and semimetals, and multiferroics, to name just a few examples. After a spectacular century-long endeavor to discover and understand quantum phenomena in materials, starting with the discovery of superconductivity in 1911, these efforts will continue to provide the foundation for new electronic

and information processing technologies. These developments will depend on the asking of new questions to gain a deeper understanding of the electronic and magnetic structure of materials—questions that can only be answered using the world’s best characterization tools. Through detailed insight into electronic band structure, spin states, and the morphology of those chemical, electronic, and structural phases that determine how a material responds to external stimuli, we gain an understanding of the material's functionality. For example, efficient computing relies on being able to transport electronic information along conducting channels and to process information in electronic gates reliably and at a minimal power cost. Measurements of the band structure and electronic excitations provide information about electrons participating in conduction and about loss mechanisms that reduce the efficiency and reliability of the operation of a device.

Many currently studied materials exhibit emergent behavior—the appearance of unexpected electronic properties and long-range ordered electronic phases. These properties often go beyond the scope of established theories and cannot easily be predicted from the properties of their individual building blocks. For example, cuprates exhibit high-temperature superconductivity, which is relevant for lossless power transmission; manganese perovskites produce complex magnetic and electronic phases that can be utilized in information storage and spintronics applications; and molecular materials offer spin and electronic states that can be switched with unprecedented energy efficiency. A recently discovered “zoo” of topological phases that exhibit unique band structures with symmetry-derived protections against scattering and many-particle interactions may become useful in new electronic devices (Fig. 1, top).

To advance the discovery of new materials with novel properties, synthesis needs to be closely integrated with knowledge of the structure and properties of the synthesized material. The ALS offers a comprehensive set of tools to both synthesize materials as well as determine these properties—tools such as angle-resolved photoemission spectroscopy (ARPES) for electronic structure measurements, x-ray magnetic circular and linear dichroism (XMCD + XMLD) spectroscopy to determine chemical and magnetic properties, photoemission electron microscopy (PEEM) to study spatially inhomogeneous and patterned electronic and magnetic domains, resonant elastic x-ray scattering (REXS) to study long-range order, resonant inelastic x-ray scattering (RIXS) to study electronic excitations, IR spectroscopy for low-energy excitations, and x-ray photon correlation spectroscopy (XPCS) to determine the temporal response of materials to adiabatic changes in temperature and external fields. Samples are grown in situ using molecular beam epitaxy, pulsed laser deposition, and micromechanical exfoliation.

The Quantum Materials Research and Discovery TA seeks to advance the discovery and understanding of new quantum materials by developing x-ray methods to measure electronic phases and orders down to nanometer length scales while pushing boundaries in regard to sensitivity, resolution, and the sample environment (temperature, fields, stress, and currents). High-priority goals (in no particular order) are the development of instrumentation and techniques for the following:

- Efficient measurements of the spin-resolved band structure of quantum materials using spin-ARPES with advanced detection schemes.
- Ultrahigh-energy-resolution (sub-millivolt) measurements of exotic electronic phases and spin textures at ultralow temperatures (sub-Kelvin).
- Magnetic microscopy of quantum materials in high magnetic fields with ≤ 20 nm spatial resolution at cryogenic temperatures.

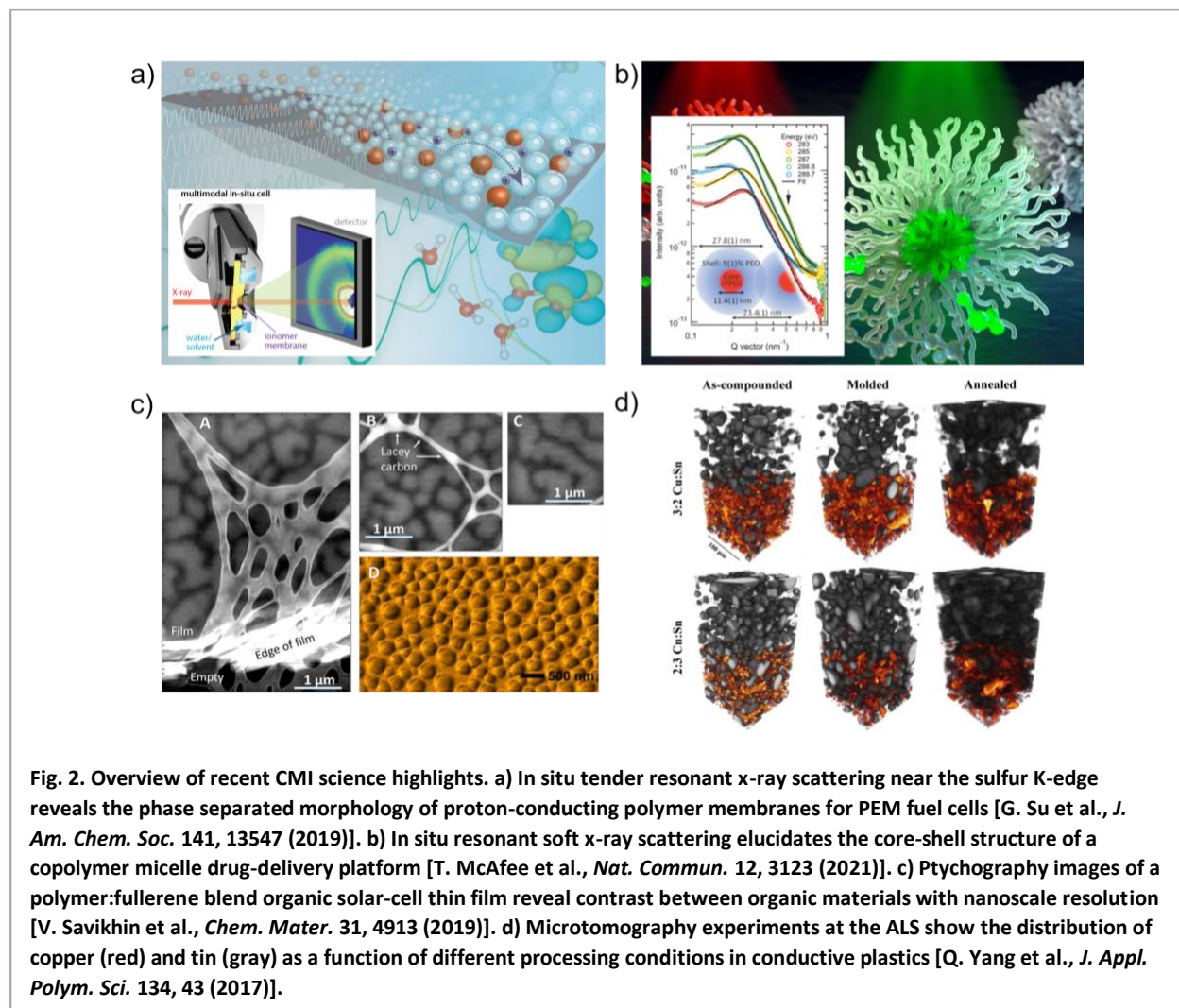
- Novel imaging modalities of elastically and inelastically scattered x-rays that can image electronic, magnetic, and other ordered phases down to nm length scales.
- XPCS measurements of electron and spin fluctuations down to nanosecond time scales.
- A novel imaging tool based on reflection geometry that will enable imaging of electronic and magnetic order and phenomena at buried interfaces and heterostructures.
- NanoARPES capabilities at the ultimate reach of spatial resolution (≤ 10 nm) for fundamentally new, direct access to 1D electronic states of single quantum objects and interface and edge states; for access to the natural length scales of electronic heterogeneity in correlated electron systems; and enabling unique sensitivity to electronic phase and coherence by probing within a material's electronic coherence length for the first time.
- Multimodal measurements combining x-ray microdiffraction and IR nanospectroscopy with soft x-ray tools together with non-synchrotron methods such as thin-film growth, atomic force microscopy, scanning tunneling microscopy, and transport tools.
- Application of tools to samples and devices under in situ/operando conditions with applied currents, strain, and electromagnetic/optical fields.

The power of these techniques will be dramatically enhanced by the improvements in beam quality delivered by ALS-U. Increasingly, ALS users seek to combine soft x-ray electronic structure techniques with other ancillary tools like scanning probe microscopies, x-ray diffraction (Fig. 1, bottom left) and synchrotron infrared nanospectroscopy (SINS) (Fig. 1, bottom right). Such multimodal methods will enable a broader and more detailed understanding of the role of heterogeneity in novel functional and quantum materials, guided by knowledge of the structure and properties of the synthesized material.

2.1.2 Complex Materials and Interfaces

The Complex Materials and Interface (CMI) TA focuses on understanding how function emerges from the complex properties of intrinsically heterogeneous materials across a wide range of length and time scales, with a particular focus on soft materials and hybrid organic-inorganic systems. Whether bottom-up grown, top-down engineered, or naturally heterogeneous, materials used in applications that include fuel cells, batteries, and solar cells are of critical importance to our energy future. In such hierarchical systems, atomic- and molecular-scale function relies on the chemical composition and crystal structure, while at the mesoscale, physical and chemical functionalities depend upon the diffusion and transport of electrons, spins, and ions through the material and across interfaces and phases. Hierarchical systems, for example, a proton-conducting fuel-cell membrane, require molecular arrangements over a range of length scales for efficient charge transport. The ALS provides a range of scattering, microscopy, and imaging tools that allow researchers to determine the electronic, chemical, and physical structure of such hierarchical systems. Scattering and diffraction techniques offer statistical sensitivity to the morphology and chemical states of multiphase systems, such as a phase-separated, proton-conducting polymer membrane (Fig. 2a), across a wide range of length scales from Ångströms to hundreds of nanometers. Element and chemical specificity provided by the near-edge x-ray absorption fine structure allows scientists to differentiate between different chemical components (Fig. 2b) and molecular orientations, which together provide key information about the relationship of structure and function. Furthermore, scanning transmission x-ray microscopy (STXM) and ptychography can, for instance, quantify nanoscale ion currents in a model system of a lithium-ion battery or domains in an organic solar cell active layer (Fig. 2c). At longer length scales, computed tomography visualizes micron-scale and

larger functional components—for example, the distribution of metal filler particles in a composite conductive plastic (Fig. 2d)—and is an excellent tool for both academic and industry users to study the 3D morphology of composite materials, metallic or ceramic compounds, and biological systems.



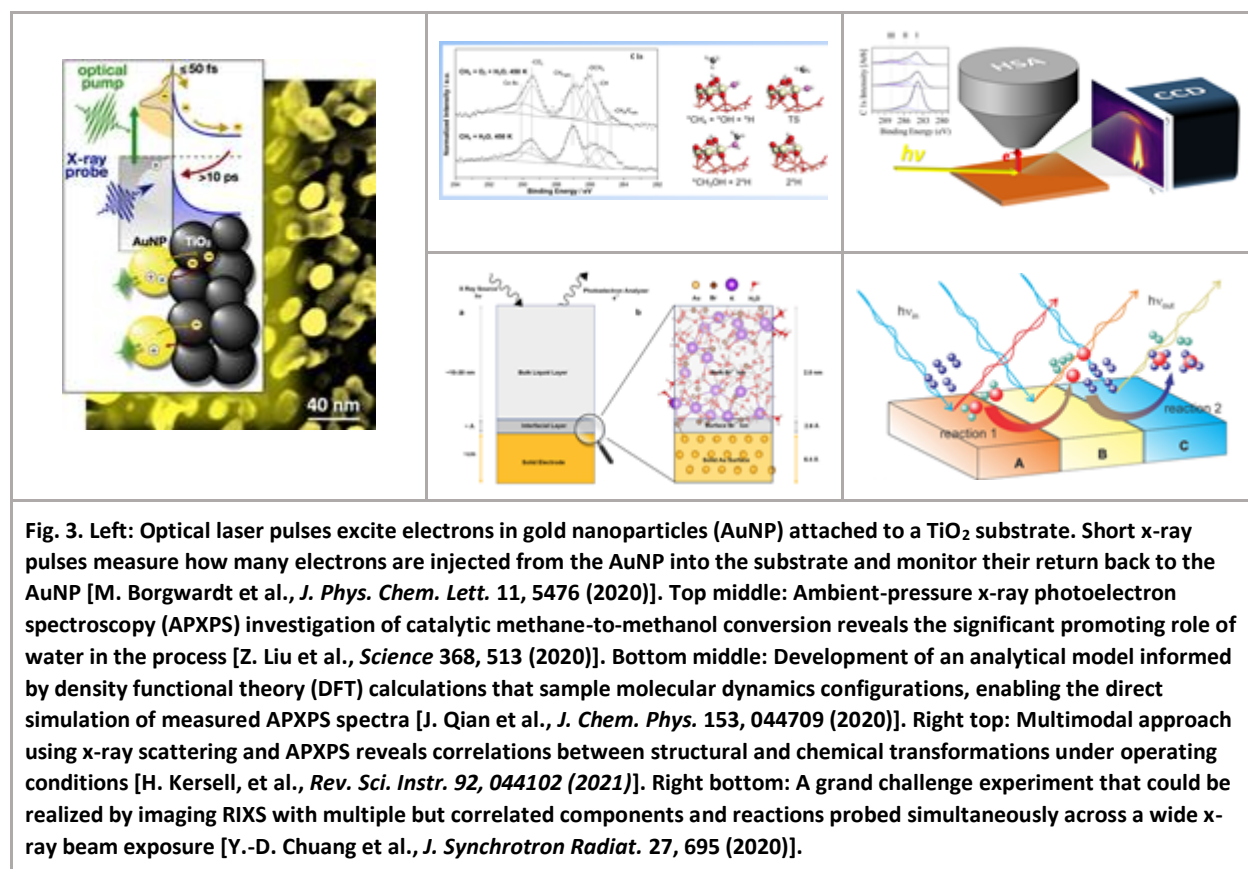
The ALS has pioneered the development of small- and wide-angle x-ray scattering (SAXS/WAXS), resonant soft x-ray scattering (RSoXS), and tender resonant x-ray scattering (TRexS) capabilities. The higher flux of an ALS-U high-field bending magnet port would enable high-throughput SAXS/WAXS measurements and access to faster time scales, and launching such an upgrade is a high priority for the CMI TA. Moreover, this TA seeks to develop internal and external collaborations that further the use of tender x-ray scattering capabilities. The CMI TA's scientific goals span hydrogen, water treatment, polymer upcycling, and energy storage, which will provide the basis to nucleate and grow a strong user community that will transition to the coherent ALS-U tender beamline. The RSoXS program is continuing to evolve and prepare for future energy-resolved chemical x-ray photon correlation spectroscopy (C-XPCS), which has the potential to monitor the dynamics of specific microphases in hierarchical materials. High-priority goals in the next few years are the development of new instrumentation that will exploit the capabilities of the upgraded ALS to address new science currently out of reach. The high brightness

of the ALS is crucial to reaching nanometer-scale resolution using techniques such as ptychography and to reaching milli-, micro-, and nanosecond time resolution using XPCS. Specifically, the development of tender x-ray techniques for the upgraded ALS will be the top priority for the CMI TA in the next five years.

- Tender x-ray microscopy will enable operando and multimodal studies of materials with high spatial resolution (<10 nm) and chemical specificity. The ability to quantify morphology and chemical or crystalline phases at high spatial and time resolution will advance many areas of science. A proposed microscope for the ALS-U tender x-ray beamline will be based on the revolutionary Nanosurveyor2 instrument of the COSMIC microscopy beamline, optimized for use at higher photon energies. Nanosurveyor2 provides world-leading spatial resolution and scanning speed in a compact and ultra-stable assembly. The new microscope will be compatible with commercial or custom operando sample environments, use state-of-the-art detectors for fluorescence detection and coherent x-ray scattering, and seamlessly facilitate correlative measurements with other microscopes.
- Novel instrumentation for tender x-ray scattering will enable studies of a broad range of materials relevant to soft matter, geo-environmental science, and bio-inspired materials. A proposed endstation at the ALS-U tender x-ray beamline will perform static characterization through resonant scattering in the 1–5 keV energy range and will offer unique access to a broad range of elemental absorption edges including Na, Ca, P, S, Si, and Ti, providing information on bond orientation or charge/orbital order with chemical specificity. One major focus of the endstation will be studies of spatio-temporal behavior using XPCS. XPCS will shed light on spontaneous fluctuations over time scales ranging from microseconds to seconds. Access to such time scales is important for studying how hierarchical systems with structures at multiple length scales evolve over time and their relation to material performance. The proposed endstation will have SAXS capabilities, x-ray diffraction at higher scattering angles, and x-ray reflectivity geometries. Furthermore, the energy tunability of this beamline will enable complementary x-ray absorption spectroscopy measurements needed to inform XPCS and resonant scattering experiments. Modular sample environments will be developed to enable in situ and multimodal approaches.

Current experimental characterization often lacks effective feedback to materials synthesis, and operando measurements remain challenging. Furthermore, advanced analysis supported by artificial intelligence and machine learning (AI/ML) is needed to decipher high-throughput experiments and multimodal measurements. Advancing multimodal studies is a long-term goal of the CMI TA—for example, seamlessly combining electron microscopy and soft/tender x-ray scattering/spectroscopy. In situ probes also inform advanced manufacturing processes. The CMI TA aims to merge automated sample handling, high-throughput data acquisition, data compression, data visualization, and data analysis techniques and strategies developed together with partners, including the Center for Advanced Mathematics for Energy Research Applications (CAMERA), the National Energy Research Scientific Computing Center (NERSC), and the LBNL Information Technology Division.

2.1.3 Chemical Transformations



Devices currently in use or being developed for selective and efficient heterogeneous catalysis, photocatalysis, energy conversion, and energy storage rely heavily on diverse multiscale phenomena, ranging from interfacial electron transfer and ion transport occurring on nanometer and picosecond scales to macroscale devices that operate on time scales of seconds to hours. Soft and tender x-ray beamlines with innovative scientific instrumentation and operando capabilities can probe dense environments with atomic and chemical contrast spanning a large spatiotemporal range and can detect correlated and inhomogeneous components simultaneously through advanced large-area imaging techniques, thereby providing unique fundamental information about these functioning mesoscale chemical devices. The utilization of hard x-rays in operando conditions contributes complementary quantitative structural and morphological information at length scales ranging from the atomic (a wide variety of x-ray diffraction techniques) to the nanometer (SAXS) to the micrometer (tomography) and has the potential to probe kinetic properties at millisecond to hour time scales. Such "micro- to nano-kinetic" measurements under operando conditions are essential to optimizing complex multiscale chemical and electrochemical devices. We aim to integrate these experimental multimodal spectroscopic capabilities with computational modeling techniques to develop complete models of chemical processes.

The Chemical Transformations TA focuses on studying the kinetics, energetics, and products of chemical reactions and transformations in diverse environments, ranging from ultrahigh vacuum (UHV) to ambient and even higher pressures, in the presence of liquid and solid interfaces and homogeneous and

heterogeneous catalysts. X-rays can penetrate chemical reactors, liquids, and gas-phase environments, and provide very specific chemical and molecular information about the catalysts, reactants, and products participating in a chemical reaction. The high brightness of the upgraded ALS will enable the study of micro- and nanoscale systems with high temporal resolution in order to follow a chemical process in real time.

High-priority goals are as follows:

- Increased access and improved capabilities for users of high-brightness tender x-rays, which would facilitate in situ/operando ambient-pressure x-ray photoelectron spectroscopy (APXPS) experiments and sub-nm-length-scale x-ray scattering experiments at higher operating pressures and providing deeper probing depths.
- Development of imaging RIXS instrumentation to realize microscopic experiments across a large area with spatial and temporal resolutions down to the nanometer and nanosecond scales. Such instrumentation would enable the simultaneous detection of correlated chemical reactions with high spatial and time resolution.
- To address chemical dynamics and reactions in liquid environments by developing a dedicated combined APXPS and RIXS setup with microseconds to seconds temporal resolution and specificity to bulk and surface properties.
- Development of a suite of state-of-the-art, multimodal techniques deployed at bend-magnet beamlines advancing our scientific capabilities for probing interfacial chemistry, in particular for probing beam-sensitive chemistries:
 - APXPS research combined with an IR port would enable new multimodal science that simultaneously probes chemical states and vibrational dynamics.
 - Fast x-ray absorption spectroscopy in transmission (FAST) combined with ML would enhance the science of chemical transformations and materials discovery through new knowledge, synergy with other experiments, and materials projects.
- Realizing high-pressure soft x-ray spectroscopy experiments for in situ/operando studies of high-pressure chemistry in energy devices. Soft x-ray experiments typically require a UHV environment, but recent ALS innovations have shown that it is possible to host the samples in localized high-pressure conditions for soft x-ray experiments. It is anticipated that liquid-flow systems can operate under 10–250 bar pressure for soft x-ray absorption spectroscopy and RIXS experiments, and preliminary tests have been performed on hydrogen storage materials under H₂-pressures of 5–10 bar.
- Development of a unique high-resolution RIXS tool (<5 meV) in the 100–200 eV region for heavy elements and critical materials studies.

2.1.4 Earth and Environmental Systems

Earth and environmental scientists use IR, soft x-ray, and hard x-ray beamlines at the ALS with high 2D and 3D spatial resolution and chemical sensitivity to disentangle complex processes in Earth and environmental systems. Capturing these processes in situ under environmentally relevant conditions of temperature, pressure, composition, and pH, with some degree of time resolution, while moving these studies toward 3D and 4D datasets, has become critical. One such example is processes that govern the distribution and chemical speciation of toxic metal pollutants in mine tailings for decontamination purposes. Complex, multimodal, in situ capabilities combining extreme pressures and temperatures and

variable compositions (including variable atmospheric environments) enable core ALS research in mineralogy and geophysics. Spatially resolved x-ray diffraction (XRD) in a laser-heated diamond-anvil cell elucidates the stability, sequestration mechanisms, and reaction pathways of volatile phases such as CO₂ or H₂O within the geochemical context of planetary interiors. Laue microdiffraction enables the discovery of new minerals (e.g., ognitite and tamuraite), and 2D-strain maps based on Laue microdiffraction enable the recovery of paleo-strains in rocks at the micron scale (Fig. 4a), which provides a quantitative understanding of rock deformation, with implications for seismogenesis and mountain building. Hard x-ray microtomography allows 3D imaging of geological samples at the micron scale, such as pore spaces and their connectivity in oil- and gas-hosting shales or characterizing the texture of pyroclastic fragments to understand volcanic eruption types (Fig. 4b). Micro-x-ray fluorescence imaging and x-ray absorption spectroscopy (XAS) in the hard and tender x-ray energy ranges enables a wide array of environmental research, notably in ocean geochemistry, metal hyper-accumulating plants (phytoremediation), aerosols and soils (climate change), critical minerals (rare earth elements and phosphate minerals), contaminated groundwater systems, and biomineralization (Fig. 4c), using sample cryogenic cooling, flow cells, and other sample environments. Finally, soft x-ray nanoprobe such as STXM are frequently used to investigate minerals/organic matter in soils, marine particles, and environmental aerosols. PEEM enables the characterization of meteorites and growth mechanisms of nanoscale precursors of biominerals. Lastly, IR spectromicroscopy is frequently deployed for the study of meteorites and other space sample returns like interplanetary dusts.

A common thread running through most of the cutting-edge research activities in the Earth and Environmental Systems TA (EESTA) is a move from static postmortem studies to time-resolved and/or in situ/operando/in vivo studies. The high penetration capabilities of hard x-rays, and to some extent IR light (with diamond windows), makes these two probes central to these developments. Furthermore, Earth and environmental systems are hierarchical over a range of length scales. Structural, chemical speciation, and elemental distribution can be determined with high spectral resolution and detection sensitivity using high-brightness x-rays. Because of their higher penetration and sensitivity to the major elements present in Earth's crust minerals, tender x-rays (1–5 keV) from a high-brightness ALS-U insertion device are also of particular interest for this TA. Following the ALS upgrade, the microprobe program will be transferred to the future Tender beamline fluorescence nanoprobe, and driving this project forward is one of the priorities of the EESTA. The future Tender beamline fluorescence nanoprobe is expected to reach nine out of ten elements that constitute the Earth's crust. Focuses of the EESTA will include developing a correlative and multiscale approach between x-rays and electron microscopy techniques aiming at understanding the structure and function of microbial communities in metal-contaminated environments, characterizing biogenic materials, and elucidating the local structure of clays using soft x-ray nano-spectromicroscopy and hard x-ray microprobe techniques in cryogenic conditions.

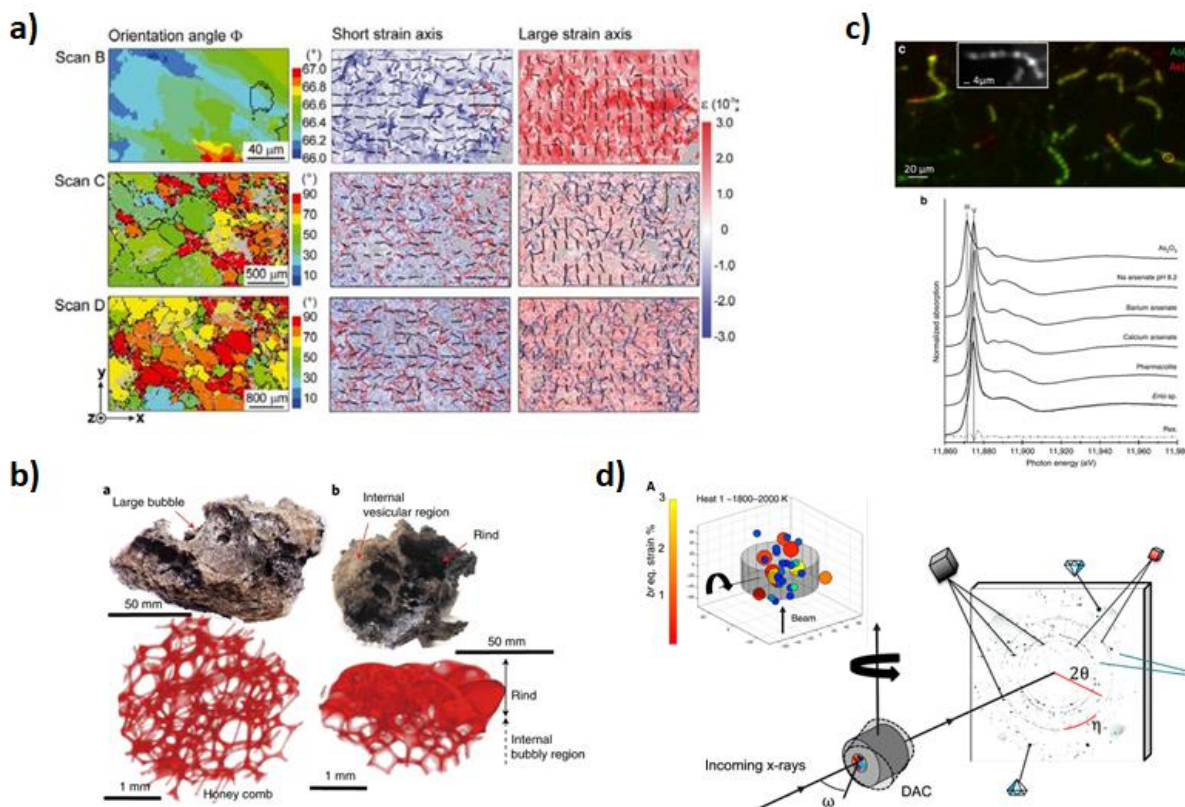


Fig. 4. a) Maps derived from Laue microdiffraction, displaying orientation (first column) and strain tensors (second and third columns) of deformed rocks from Belgium [K. Chen et al., *Geophys. Res. Lett.* 43, 6178 (2016)]. b) Vesicular pyroclasts with unbroken and reticulite-like fractured regions (top). X-ray microtomography of fragments to examine their texture, providing insights on vesiculation and volcanic gas cooling processes (bottom) [A. Namiki et al., *Nat. Geosci.* 14, 242 (2021)]. c) X-ray fluorescence elemental (inset) and chemical maps of arsenic in sponge-associated filamentous bacteria (*Entothoonella* sp.) at 95 K (top) and arsenic K-edge XANES (95 K) of *Entho.* sp. (LSQ fit 47% sodium arsenate, 39% pharmacolite and 14% As_2O_3) demonstrating that this bacterium mineralizes As(V), suggesting it acts as a detoxifying organ for the sponge (bottom) [Keren et al., *Nat. Comm.* 8, 14393 (2017)]. d) Schematic and main result of a multigrain XRD experiment in a diamond anvil cell. The multigrain technique bridges the gap between a perfect single crystal and a perfect powder, allowing quantitative determination of orientation and the spatial relationship between several individual grains (up to ~ 100) originating from a pressure- and temperature-driven phase transition or chemical reaction [B. Chandler et al., *Science Adv.* 7, eabd3614 (2021)].

Research in Earth and environmental sciences in the US is funded by several separate federal agencies, including DOE, the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), and the US Geological Survey (USGS), with by far the largest amounts being contributed by NSF and NASA. This broad federal funding represents a tremendous opportunity for the ALS, since it not only allows the ALS to contribute to a very broad range of geoscience research beyond the scope of DOE-BES priorities, but it also offers opportunities to raise supplemental funding for research and development from outside the DOE budget. An illustrative example is the NSF-funded Consortium for Materials Properties Research in Earth Sciences (COMPRES), which has contributed to ALS operation and beamline development since 2003 by funding hardware and two full-time beamline staff. For this reason, the EESTA is seeking and fostering contacts and collaborations not only within LBNL's Earth and Environmental Sciences Area (e.g., through the National Alliance for Water Innovation

(NAWI) Innovation Forum, Berkeley Lab's Carbon Negative Initiative, and Charter Hill strategic planning), but also outside the DOE complex among NSF-, NASA-, and USGS-funded PIs and organizations. Such an inclusive approach will help ALS beamlines with a focus on Earth and environmental sciences to participate in a variety of recent and anticipated funding opportunities from within DOE (e.g., carbon reduction and critical minerals) and outside DOE (e.g., NSF's Earth in Time vision and NSF's Division of Earth Sciences program solicitation for a synchrotron community facility).

High-priority goals for this TA include the following:

- Develop cross-platform sample environments for measurement of materials under in situ (e.g., cryogenic)/operando conditions using IR, spectromicroscopy, scattering, and diffraction techniques.
- Expand in situ capabilities in terms of P-T-atmospheric/liquid conditions and time resolution to offer appropriate tools to respond to DOE's carbon mineralization and critical mineral priorities. Expanding cryogenic spectromicroscopy capabilities will be crucial to address these two areas.
- Optimize and expand existing measurement facilities across the spectrum for collaborations and general use to address NSF's Earth in Time decadal report and vision.
- Drive the science case and specifications for the new ALS-U Tender nanoprobe, including educating the community, acquiring funding, and performing R&D.

2.1.5 Biosciences

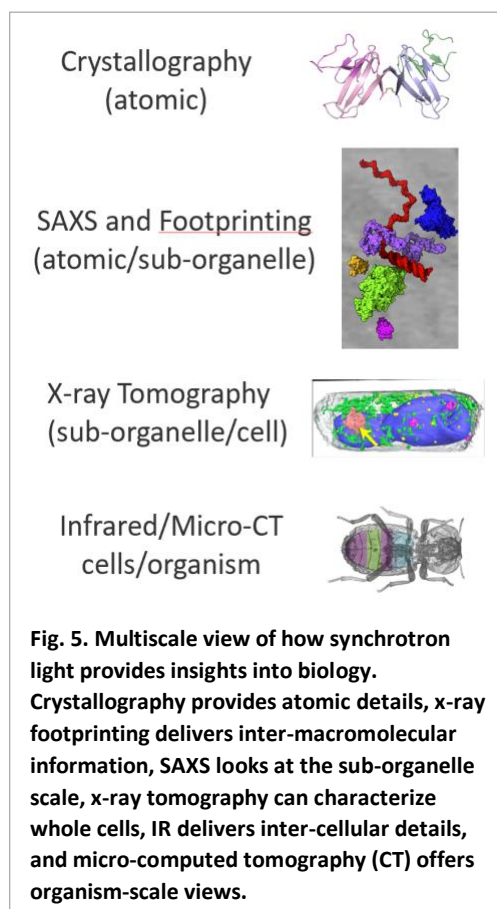
Over the next five years, the ALS will continue to provide unique opportunities to address and respond to national priorities such as climate change and human health, exemplified by the COVID-19 pandemic. Key to the ALS impact to these global challenges are strong and vibrant programs in biology. With the synergy of Biosciences TA (BioTA) capabilities with other regional resources, LBNL is exceptionally positioned to address these and other pressing topics (e.g., diseases, biofuels, and biomaterials).

Most of the BioTA-related programs receive funding external to the ALS and rely on Participating Research Team (PRT) beamlines. BioTA is a forum for ALS and PRT scientists to develop a common strategy for biosciences at the ALS. An immediate challenge the BioTA must address is preserving funding through the ALS-U Project and coming out stronger after the ALS-U dark period. The BioTA is seeking ways to take advantage of the ALS-U dark period to upgrade its resources and make use of the higher-brightness light provided by the upgraded ALS. The BioTA will work aggressively with the ALS to ensure every program has an upgrade plan and exits out of the ALS-U Project with new and improved capabilities.

Some of these activities have already begun. The Gemini macromolecular crystallography (MX) beamline, managed by the Berkeley Center for Structural Biology (BCSB), is funded to develop one, and likely two, branchlines with a view of what will be possible with the upgraded ALS. Brighter beams will enable the collection of better data from smaller crystals. ALS-U high-field bends are somewhat softer but much brighter than ALS superbend magnets, and optics optimized for ALS-U could more tightly and efficiently focus the light at MX beamlines in Sectors 4, 8, and 12. Initial R&D to develop upgrade plans has begun. The Structurally Integrated Biology for Life Sciences (SIBYLS) SAXS beamline staff are developing plans to upgrade their endstation and perhaps reduce the optimized experimental energy to

better overlap with ALS-U optima. For larger spatial scale imaging, building laser-induced fluorescent-based capabilities to be deployed side-by-side with x-ray tomographies on the same samples will greatly enhance the x-ray tomography programs and provide information even during the ALS-U dark period. These latter activities are currently unfunded, and finding appropriate funding sources must begin.

The collective BioTA can help each of its members plan, fund, and execute an upgrade plan through integration into a multiscale view of biology (Fig. 5). Crystallography provides atomic details, x-ray footprinting delivers inter-macromolecular information, SAXS looks at the sub-organelle scale, x-ray tomography can characterize whole cells, IR delivers inter-cellular details, and micro-computed tomography (CT) offers organism-scale views. In addition, several of these techniques are capable of describing overlapping temporal mechanisms. To enhance this multiscale asset of biology at the ALS, the BioTA will seek projects that apply all techniques to a related system, connecting atomic- to organism-scale phenomena. Biofilms and plants are natural targets for cross-beamline applications and address climate and health areas.



To further enhance BioTA science, we will be looking to support programs at the Joint Genome Institute (JGI), the Joint BioEnergy Institute (JBEI), the Molecular Foundry, and the University of California (UC), Berkeley. These world-class institutions study important systems that the BioTA can uniquely inform. The BioTA will serve to broaden the application of each individual technique and extend studies to new scales for more impactful results.

2.1.6 Instrumentation and Computing

The Instrumentation and Computing TA comprises instrumentation experts; beamline scientists; computing, networking, and AI and ML experts; and partners who advise the ALS about instrumentation R&D opportunities. Facilitating world-class scientific research at ALS beamlines requires continuous, strategic investment in critical technologies that push boundaries and overcome current limitations in experimental capabilities. The most important capabilities to be developed have been identified by the Instrumentation and Computing TA to be the following:

- Raise the quality of beamline optics and instrumentation to meet the requirements set by the orders-of-magnitude gains in coherent power from the planned ALS source upgrade.
- The development of in situ and operando sample environments, with an emphasis on multimodal experiments on multiple beamlines.

- The automation of experiments to enable more complex procedures, efficiently use the very limited resource of beamline scientists, and enable remote operations to reduce the burden on users.
- The development of ML and AI support for efficient discovery and understanding from multimodal spectroscopy, tomography, and scattering experiments.
- The direct linkage of theory with experiment at the beamline through the development of digital twins.
- An agile strategy to advance network, computing, and IT safety/security technology at beamlines to enable scientific goals.

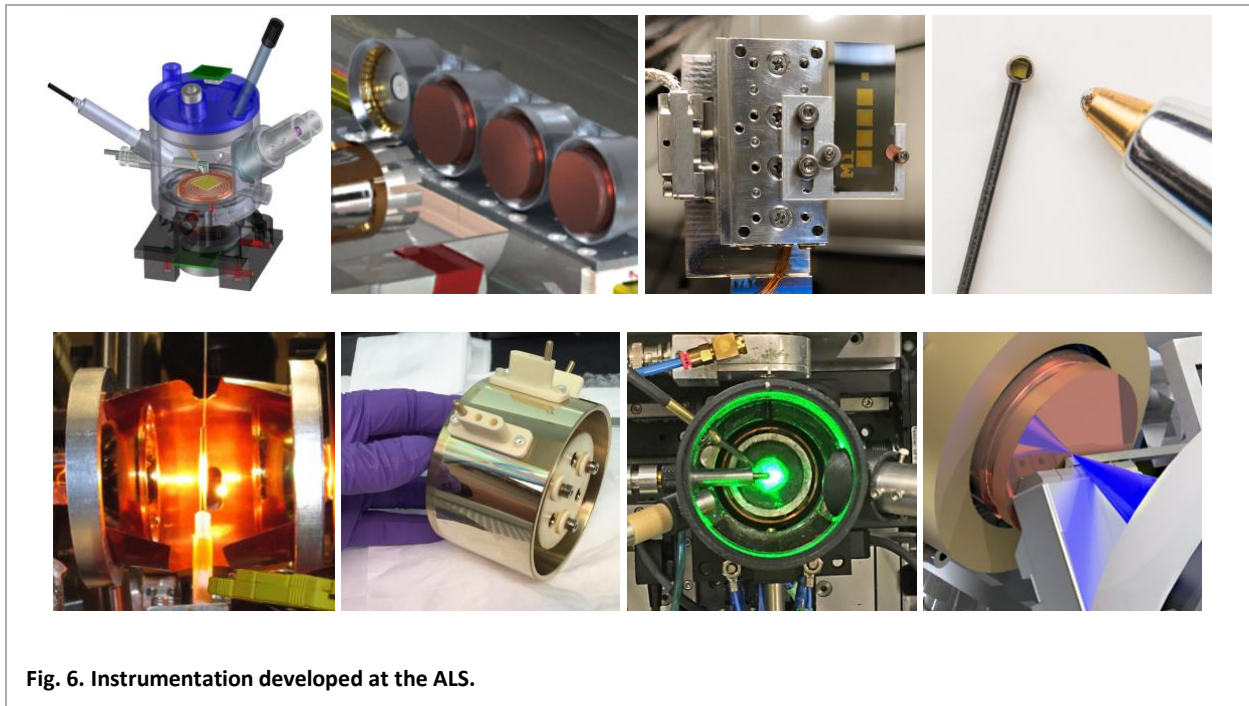


Fig. 6. Instrumentation developed at the ALS.

Beamline optics and Instrumentation. Beam diagnostics, including beam-position and energy monitors and wavefront sensors, provide essential feedback for the creation of stable, high-coherence beamlines, and they can reduce the maintenance downtime of existing beamlines. We envision the advent of common, multifaceted diagnostic tools, tailored for soft and tender x-ray beamlines and incorporated into new designs or retrofitted onto existing systems.

Adaptive optics for wavefront correction and beam shaping is emerging as an available technology with deployment and refinement taking place at several facilities worldwide. With nanometer-scale surface control becoming possible, we believe that integrated adaptive elements will be required to preserve beam properties in the most demanding beamline applications. Coupled with wavefront-sensing feedback and driven by AI-based algorithms a full implementation of adaptive elements at soft and tender x-ray energies will require the development of reliable, automated control systems. Furthermore, mirror metrology is a foundational technology that has enabled the creation of optical elements in x-ray optical systems of diffraction-limited quality. Advances in mirror quality follow improvements in metrology, which occur through innovative instrumentation and fastidious attention to

systematic errors. Despite significant advances, metrology is challenged to exceed accuracy levels much below 50 nrad.

In situ and operando sample environments. Operando multimodal sample environments are of utmost importance for collaboration-driven science at the ALS. Specifically, we need to develop in situ, multimodal probes to interrogate materials when they are evolving or out of equilibrium.

Many complex materials require the use of multiple techniques. To investigate the intricacies of perovskite solar cells, for example, it is important to be able to perform x-ray scattering, IR, and photoluminescence experiments in situ during the spin-coating process. The dynamics of novel devices for quantum information science (QIS) occur on a hierarchy of length scales that cannot be captured just by integrative transport measurements. New tools are required that directly probe the order and dynamics of charge carriers in such devices at the crucial length scales, in their natural habitat, with current flowing and wires attached. Making such sample-modification environments available with multimodal approaches will drastically increase the impact of existing ALS beamlines.

Furthermore, ALS beamlines offer a variety of structural, chemical-state, magnetic, and electronic imaging techniques using light from infrared to hard x-rays. Powerful insights arise from combinations of these tools, enabling researchers to probe complex functional relationships. This is especially true for inhomogeneous samples with either engineered or spontaneous heterogeneity. In such complex samples, the direct correlation of diverse properties, determined at fixed sample positions under controlled conditions (e.g., a gaseous environment or applied field), will be immensely more valuable than if applied to multiple similar, non-identical samples. Currently, the coordination of multiple beamlines to achieve this type of measurement is hampered by instrumentation challenges—the lack of compatible sample holders, challenges in preserving sample environments between measurements, and diverse file formats and data-logging systems.

Experiment automation. Increasing automation will enable a cohort of new possibilities for experiments at the ALS:

- The ability to run experiments remotely.
- A drastic increase in scientific output capacity due to the ability to run experiments more efficiently and without human intervention necessary at each step.
- Advanced planning of experiments, leading to a more efficient use of beamtime.
- The ability to take advantage of AI/ML to drive autonomous experiments.
- The ability to reliably capture metadata about experiments, leading to more “FAIR” data (findable, accessible, interoperable, reusable).
- Better reproducibility of experiments.
- Reduction in human error during experiments (especially relevant for experimental campaigns that often require long, overnight hours).

For all these reasons, increasing automation is a key priority. Significant work is required to build robust automated systems, both in hardware and software. Hardware includes robotics and computer-controlled motors and actuators, along with sensors and cameras that work together reliably. Software includes systems that allow end-to-end tracking of samples (including samples shipped to and carried

onsite), sample changing, alignment, and comprehensive recording of beamline and instrumentation parameters.

Historically, most work toward automation has been done at the protein crystallography beamlines. At those beamlines, every sample has a common mount and every experiment is similar in terms of approach to alignment and scanning. These have been ideal beamlines to automate. Automating other beamlines poses challenges due to the greater variety in the size/shape/type of samples, different sample environments, sample mounting strategies, and other setup parameters. Driven by the need to enable more remote access, the ALS is working to develop a more specific automation plan that gauges the challenges and the benefits of automation at each of its beamlines and prioritizes development of automation at each.

Rather than leaving the design and deployment of automation to each beamline scientist, our strategy will be dedicating specialists to developing hardware and software systems that can be adapted and deployed across beamlines. This work should leverage the development that has been done by several beamlines and will also coordinate with work being done at other facilities.

Community-focused machine learning and artificial intelligence for the ALS.

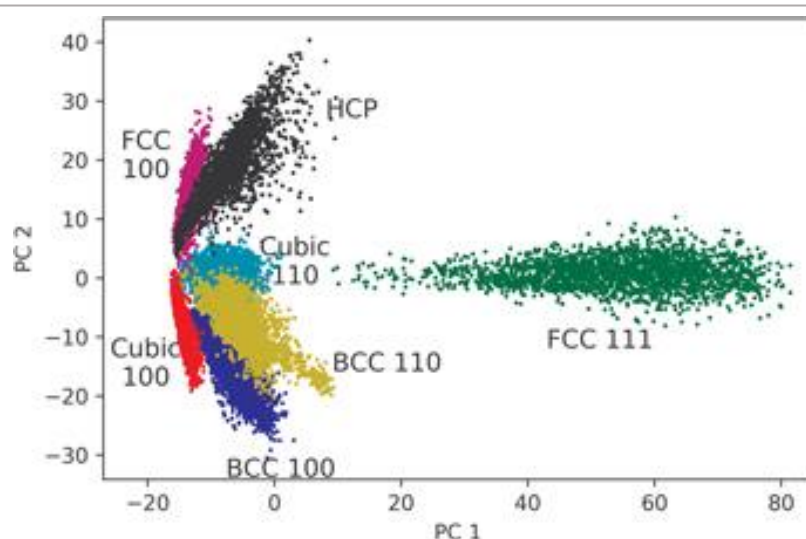


Fig. 7. Convolutional Neural Networks classification of nanoparticle orientation in a thin film learned by grazing-incidence SAXS (GISAXS) patterns. The network was trained on thin films with a success rate of 94% [S. Liu et al., *MRS Communications* 9, 586 (2019)].

There is tremendous potential in using AI and ML techniques for coordinating complex experiments and data analysis. AI/ML can aid in building reproducible science, optimize the use of experimental facilities, increase transparency, and widen the pool of available knowledge, allowing us to find and illuminate intricate scientific relationships inherent in the collected data. Advances in scientific machine learning offer an opportunity to leverage the commonalities, scientific insights, and collected experience of the larger scientific user facility community. Taking advantage of this community will enable an integrated view that maps the broader scientific context and delivers an aggregate view of the strengths and weaknesses of the field as a whole. The ALS focuses on developing community-driven AI/ML tools to aid user-facility scientists and users. Realizing the benefits of cross-facility AI/ML efforts requires enhancements to beamline data-acquisition systems, metadata databases, and data-storage systems.

Acquisition systems that can integrate with software frameworks that are common to data science will help bring AI to the beamline directly. Feeding metadata databases with beamline information as it is captured will allow users take advantage of AI and ML tools during analysis.

Digital twin. A digital twin (DT) is defined as an in silico simulation of an in situ and operando experiment that can simulate outcomes, investigate failure modes, or rapidly prototype and test protocols at ALS beamlines. Our goal will be to expand the integration of theoretical and experimental exploration into DT of systems of interest, for example, chemical processes at solid/gas, solid/liquid, and solid/solid interfaces, or in studies of the role of defects on correlated states of superconductors, topological states, or quantum coherence. The DT will provide robust feedback between material and chemical synthesis, experiment, and theory driven by AI/ML. This effort will advance our ability to probe and understand emergent phases and dynamics that arise across fields when there are many configurational degrees of freedom and when competing interactions with comparable length and energy scales are involved. These innovations can significantly accelerate new scientific discoveries beyond what we would traditionally accomplish by comparing experiments to established theoretical insights and numerical simulations.

Computing. The beamline information technology (IT) infrastructure needs to be updated to support changes in the way science is performed at the ALS. Currently, the IT system is very open and many IT decisions are left up to the beamline scientists. This poses some problems. Control systems should not be exposed to the internet at large. Data-management tools developed for one beamline are fairly network dependent and cannot easily be applied to other beamlines. Remote work will become more popular and requires better security planning. Multi-beamline and multi-facility measurements are currently hampered by decentralized storage of experimental data and metadata. The ALS is studying how new infrastructure at beamlines could meet these challenges before and after ALS-U.

2.2 ALS Upgrade and long-range accelerator planning

ALS-U is an ongoing major upgrade of the ALS that will endow the light source with revolutionary x-ray capabilities. The ALS has been a global leader in soft x-ray science for more than two decades. Recent accelerator physics and technology breakthroughs now enable the production of highly focused beams of soft x-ray light that are at least 100 times brighter than those of the existing ALS. Applying this technology at the ALS will help us to better understand and develop the new materials and chemical systems needed to advance our energy, economic, and national security needs in the 21st century, securing the United States' world scientific leadership for decades to come.

The upgraded ALS will occupy the same facility as the current ALS, replacing the existing electron storage ring and leveraging about \$500 million in existing ALS infrastructure, accelerators, and experimental systems. The new ring will use powerful, compact magnets arranged in a dense, circular array called a multibend achromat (MBA) lattice. In combination with other improvements to the accelerator complex, the upgraded machine will produce bright, steady beams of high-energy light to probe matter with unprecedented detail.

The improved capabilities of the upgraded ALS at new and upgraded beamlines will enable transformative science that cannot be performed on any existing or planned light source in the world. This new science includes 3D imaging with nanometer-scale spatial resolution and measurement of

spontaneous nanoscale processes with time scales extending from minutes to nanoseconds—all with sensitivity to chemical, electronic, and magnetic properties. Moreover, the beam’s high coherence will enable new classes of optical techniques that will provide the groundbreaking sensitivity and precision needed to detect the faintest traces of elements and subtle electrochemical interactions on the scale of nanometers.

The upgraded ALS is designed to be unsurpassed by any currently envisioned technology and will enable world-leading soft x-ray science for years to come. In June 2016, BESAC released the recommendations of the BES Facility Upgrade Prioritization Subcommittee, whose report deemed the ALS-U project “absolutely central” to contribute to world-leading science and “ready to initiate construction”—the highest possible ratings in the prioritization process. In September 2016, DOE initiated the ALS-U project by approving its “mission need” and assigning it CD-0 status, the first milestone in making ALS-U a reality. In December 2019 the project received CD-3a approval (long-lead procurement), and in April 2021 it achieved the CD-2 milestone (approved performance baseline).

In order to support the operation of the present and upgraded ALS for an additional several decades, a multi-year prioritized plan for upgrading/replacing legacy accelerator facility subsystems and components was initiated several years ago and will continue in the future. A number of major subsystems, such as the booster- and storage-ring radiofrequency (rf) systems, the accelerator control systems, the timing system, and most of the magnet power supplies, the linac high-power modulators were already replaced with present state-of-the-art technologies, and upgrades of additional major systems, such as the replacement of the linac rf controls and other main systems, are planned.

In addition to these projects targeting reliability, a list of prioritized projects, focused on accelerator performance improvements, has been developed, and the highest-priority items in the list are being progressively initiated. In setting priorities, benefits for both the present and the upgraded ALS have been taken into account. Notable examples in this performance-improvement category include new high-performing, higher-bandwidth fast orbit feedback, an ML-based application for improving the stability of the electron beam size, etc.

Additional information on both project categories can be found in section 3.1.

2.3 User program, strategic planning, communications, and workforce development

2.3.1 User program and user services

The quality and impact of the ALS’s research depends on an engaged and innovative user community as well as input from other internal and external sources. In collaboration with our scientific staff, our users bring forward key ideas that fuel our facility. As such, our strategic plan is guided by their diverse input, which we seek on a regular basis.

- Our Users’ Executive Committee (UEC) serves as an interface between ALS staff and users. We engage them formally and informally several times per year to identify ways to help users be more productive at the facility. The UEC is elected from the user population and generally represents the spectrum of research activities at the ALS.

- The annual User Meeting is organized by the UEC and includes topical workshops and tutorials planned collaboratively by our staff and users. The meeting is well attended and provides invaluable advice on emerging opportunities and research priorities. The ALS financially supports the User Meeting in recognition of its impact on the ALS's strategic direction. The User Meeting is currently held as a virtual meeting via video conferencing.
- In addition to the regularly held User Meeting, we also convene special ad hoc workshops and town halls. The ALS Thrust Areas organize Innovation Forums for members of our community that are designed to lead to new collaborations, educate the community about new capabilities, and inform the ALS science and instrumentation strategy. Two workshops were organized by the ALS scientists developing the science and endstation instrumentation strategy for the ALS-U tender x-ray beamline, and beamline advisory teams have been formed.
- Approved Programs (APs) provide longer-term, guaranteed access to beamtime for an individual or group proposing a high-quality research program, as evaluated against the General User (GU) population. AP proposals are evaluated by the Proposal Study Panel (PSP), which also evaluates regular GU proposals. APs contribute to the ALS's strategic direction by helping to develop significant new capabilities. The final recommendation on an AP proposal is made by the Scientific Advisory Committee (SAC), which also gauges the R&D plans in terms of the overall ALS program.

The ALS user services web interface is the first face of the ALS seen by ALS users. Provision of a modern user services business system, for coordination of user registration, proposal administration, beamline scheduling, safety management, and tracking and reporting outcomes, is essential to ensure safe and efficient user operations at ALS. ALSHub, the ALS user portal, provides a single point of entry to a personalized, easy-to-use interface which allows users and staff to do the following:

- Register and notify the ALS of a user's arrival date
- Track the status of user agreements, training, and ALS building access
- Submit and view current and past beamtime applications
- View the ALS and beamline schedules
- Submit and view current and past experiment safety documents
- Report and search for publications
- Complete all safety and security requirements and provide feedback to ALS
- Access a secure portal to use beamline computers remotely
- Link to LBNL human resources and foreign-visit and software applications to efficiently meet DOE requirements

Recent software developments have provided ALS users with a suite of modern and effective tools accessed through the ALSHub interface, including the ALS Scheduler (a centralized scheduling application), the Experiment Safety Assessment Form (ESAF) system to manage user experiments, and upgraded publication report and search tools. A federated identity management system has been implemented that allows users and staff to access ALSHub either using their existing LBNL, ORCID, or InCommon ID. At this point, the ALS will undertake a rolling program of assessing and, if necessary, upgrading each component to ensure that the user services system remains fit for its purpose. The ALS continues to reach out to other user facilities, both within LBNL and nationally, to develop consistent

best practices for user services software. During the next five years, it is anticipated that the ALS will do the following:

- Replace or update the current proposal administration system. We envisage the replacement product will allow users to select resources across multiple LBNL user facilities. This project will likely be in conjunction with the Light Source Common Software Committee and/or with other LBNL user facilities.
- Participate in coordinated exchange of user data, including digital identifiers such as ORCID and DOIs, to add metadata to scientific data collected at the ALS. This will be necessary to enable streamlined mechanisms of data analysis and storage. APIs to give staff targeted and secure access to User Office database information have already been developed.

2.3.2 Strategic planning



The ALS strategic planning process is designed to a) identify new opportunities in synchrotron radiation science, b) recognize and balance the instrumentation needs of our user community, and c) determine technologically advanced and cost-effective solutions to achieve ALS goals.

The ALS uses the following prioritization criteria when assessing new projects:

- Will user research enabled by the project likely have high impact and lead to transformational scientific discoveries?
- Does the project serve a strong community of users in the area of basic energy sciences?
- Will the project significantly enhance the technical capabilities of beamlines or the accelerator in support of user research?
- Is the solution cost effective, appropriate, and technically advanced?

In our planning process we utilize the expertise of the ALS scientific staff who are distinguished scientists and stay in close contact with the user community and experts in the field of synchrotron instrumentation to identify new science opportunities and develop new beamline and accelerator initiatives. ALS scientists are knowledgeable about current research trends and many serve as members of review boards at other light sources, as members of scientific planning committees, and participate in workshops and conferences. The ALS has formed TAs that are charged with incubating new ideas in strategically important areas of x-ray research. Scientists in TAs can seek ALS and LBNL internal resources, including collaborative fellowships or Laboratory Directed Research and Development (LDRD) funds, to develop these ideas. The ALS Science Council, an ALS internal review board, advises ALS management about prioritizing resources, for example for beamline and endstation projects, and supervises the ALS fellowship programs (see section 2.3.5) and the ALS Colloquium, a regularly occurring set of seminars featuring a diverse group of high-profile speakers.

The ALS SAC is composed of national and international experts from many disciplines and meets twice per year to provide high-level advice to LBNL and ALS management. The ALS strategic plan and resulting priorities are discussed in detail with the SAC. With oversight from the SAC, the ALS regularly organizes crosscutting reviews of all beamlines organized by entire subdisciplines to seek focused advice on how to optimize our capabilities to address important research problems.

2.3.3 Communications

The ALS Communications Group is responsible for highlighting the facility's capabilities and amplifying highly impactful research carried out by our users and staff to a diverse set of audiences, including current and potential users, DOE, other synchrotron facilities, and the general public. The Communications Group coordinates closely with all functional areas of the ALS to stay apprised of achievements, updates, and plans that need to be communicated to these audiences, and also plays a critical role in user communications and internal staff communications.

The ALS's primary distribution channels for news and updates include the ALS website and a monthly newsletter, ALSNews, which has over 5,000 subscribers. The group also collaborates with LBNL's Strategic Communications department to increase the visibility and reach of ALS research outputs to the media and general public. Another primary distribution channel is social media, which the ALS uses in combination with multimedia to better reach a breadth of audiences, including the general public and younger demographics. The ALS also offers online forums to apprise users of critical news and opportunities involving ALS-U and receive feedback.

The Communications Group continues to build out features on its public-facing website that make the content more accessible and to highlight capabilities and pathways for collaboration with our scientists. The group is now working with Photon Science staff to launch program websites that will complement the public-facing site by offering more detailed technical information about beamline offerings and techniques geared towards users. In addition, brief fact sheets on beamline techniques will be developed and posted to the website and printed for distribution around the ALS facility and at in-person and virtual conferences.

Another focus of the Communications Group is internal communications. ALS staff are distributed across multiple LBNL divisions and work in multiple physical locations, and at any given time there are a number of visiting scientists and users onsite as well. TV monitors placed throughout the ALS provide

updates on scientific accomplishments, upcoming seminars, and other announcements. The Communications Group maintains an intranet site that is accessible to anyone with a Lab login. The intranet comprises both dynamic and static content—an archive of timely email updates and event announcements as well as resources the staff need, including safety information, administrative guidelines, and document repositories. The recently instituted ALS all-to-all (all-staff) meetings serve as a central forum for internal communications. The Communications Group produces a summary of the main points as a text-based complement to video recordings of the meetings.

Finally, the Communications Group focuses on outreach, which encompasses students and visitors from the general public, government officials, and potential users. The ALS works with LBNL's Government and Community Relations Office and Protocol Office to host high-profile officials and other visitors, as well as to provide requested information to Congress and the California State Legislature, and to plan events on Capitol Hill. The Communications Group also provides tours and high-level overviews of the ALS to visitors invited by the Lab's K-12 and Workforce Development and Education offices, educating students and exposing the next generation of potential scientists to synchrotron career options. When appropriate, the Communications Group also connects these visitors with ALS staff, who provide a more specialized perspective on the facility. The Communications Group also offers internal tours, to allow LBNL staff members to become more familiar with the research done at our facility. In light of the pandemic, a virtual tour was developed as part of the Protocol Office's virtual LBNL public tour, reaching a global audience over video, and is likely to remain part of the ALS's outreach portfolio. The Communications Group also recently revamped an educational poster on how the ALS works and is expanding on the content by developing a web-based tutorial.

Moving forward, the ALS will continue to engage in these outreach efforts, with an increased emphasis on ALS-U and its benefits for the scientific community. As well, it will become increasingly important over the next few years for the Communications Group to recommend and support communications to users and staff around the logistical impacts of the ALS-U Project, including key project updates and impacts to user and other ALS operations. A multi-pronged strategy encompassing the ALS website and intranet, newsletters and other email distributions, virtual town halls, and in-person and other virtual meetings will be developed and implemented.

The Communications Group also works with ALS scientists to ensure that they have the outreach resources they need to attract new users. In collaboration with our scientists and User Office, the Communications Group will help develop specific outreach strategies to ensure a strong base of users who are prepared to take advantage of the enhanced capabilities of the upgraded ALS.

2.3.4 Inclusion, diversity, equity, and accountability

The ALS has a strong commitment to diversity, equity, and inclusion and supports a culture in which the entire ALS community, including staff, users, affiliates, and visitors, feels welcomed and valued.

LBNL and the ALS believe that inclusion, diversity, equity, and accountability (IDEA) are key enablers to accomplishing the Lab's vision of bringing science solutions to the world. As critical components of the Lab's stewardship efforts, they unlock innovation, produce high-performing teams, and drive meaningful impact and outcomes. LBNL and the ALS strive to

- create an environment in which everyone belongs (inclusion);

- welcome and engage all people and perspectives (diversity);
- ensure fair access to opportunities (equity); and
- take responsibility for making progress (accountability).

The ALS's IDEA framework encompasses several task forces and an IDEA Committee (Fig. 9). Task forces address a focused set of issues related to ALS culture and consist of volunteer members. The chairs of these task forces, along with the IDEA chair, an IDEA facilitator, and two at-large representatives elected annually by ALS staff comprise the IDEA Committee, which coordinates task force activities and makes recommendations on policy changes to the ALS leadership. The IDEA framework is flexible, allowing task forces to sunset or be created to address new priorities.

The IDEA Committee and its task forces are working to improve ALS policies and culture with regard to career and professional development; onboarding; recognition; recruiting and hiring; social activities; education and communication; and work-life balance. Within the past year, the ALS IDEA Committee and task forces have:

- Led a community process to refresh the ALS's mission statement and identify a set of core values
- Administered the second annual ALS climate survey and identified areas of success and areas that need improvement
- Publicized harassment and discrimination reporting policies and contact information
- Developed guidelines for LBNL Spot Awards, which acknowledge and reward outstanding individual and/or team workplace contributions that occur on a day-to-day basis
- Introduced improvements to the performance review process
- Broadened the impact of ALS-developed best practice guidelines for recruitment and hiring processes by developing Energy Sciences Area-wide guidelines in collaboration with the Molecular Foundry



Future priorities include continuing to institutionalize the ALS core values and to assess and refine improvements that have been implemented. Some specific goals for the next year include publicizing Lab-wide career development and promotion resources and programming and identifying ALS-specific areas that need improvement; recommending and implementing improvements to gender equity; tailoring the hiring guide for operations hires; developing mechanisms and guidelines for internal and external award nominations; and establishing a formal mechanism for employee-supervisor work-life balance discussions. This last point will be particularly important as the COVID-19 pandemic continues to evolve and LBNL implements flexible work options that will give many employees more leeway in their work location.

2.3.5 Fellowship programs

The success of the DOE synchrotron radiation facilities depends strongly on developing a knowledgeable and highly trained community of users and beamline scientists who apply existing and innovate new tools, often collaboratively, to pursue a diverse array of research frontiers. It is very important to

establish a strong pipeline of talented candidates to become facility staff—at the ALS and at other facilities—in the future. Aside from the user-training activities that happen daily on the experiment floor, the ALS sponsors two related programs that directly impact the professional development of young scientists, from college undergraduates to advanced postdoctoral associates:

- **ALS Doctoral Fellowship Program.** This program supports about a dozen doctoral fellows. This program is highly competitive and attracts superb young talent to the ALS. The ALS offers each Fellow stipend support of about 50% of a typical graduate student's pay. The Fellow's thesis supervisor generally provides the balance of financial support as well as university benefits. In addition to training, other goals of the program are to engage the thesis advisor deeply in ALS research activities and to provide a career-development opportunity and supervisory responsibility to ALS staff scientists. The program was established in 2003 and has developed an impressive list of alumni—some now ALS staff and users.
- **ALS Collaborative Postdoctoral Fellowship Program.** This program takes a collaborative approach similar to the doctoral program described above. The strength of the ALS in applying x-rays to frontier research problems attracts a very strong pool of applicants. The financial arrangements are more diverse than for the doctoral program, but the funds are similarly leveraged and a primary intent is again to engage the user community in strong collaborations.

The ALS Science Council oversees the fellowship programs, helping to maintain a high degree of leveraging and ensuring strong alignment of the programs with the facility's strategic plan. Applications for doctoral fellowships are evaluated once per year, and postdoctoral fellowships are evaluated quarterly.

2.4 Safety

As part of Integrated Safety Management (ISM), the ALS Safety Program continuously evaluates its effectiveness and identifies opportunities to improve. These improvements are integrated with, and support, the ALS Strategic Plan.

Accelerator and beamline safety. While safety at the beamlines is the primary responsibility of the beamline scientists, the floor operators play a key role in ensuring that beamline activities are conducted with the appropriate radiation safety controls. Accordingly, the scope of floor operator responsibilities and oversight regarding beamline operations and configuration is being enhanced through training, updated procedures, improved communications, and expanded roles. A lead floor operator position has been created to assist the operations supervisor in accomplishing these tasks. The radiation safety program at ALS is overseen by the radiation physicist, who works in conjunction with floor operators, review committee chairs, and technical groups to protect people from harmful effects of exposure to ionizing radiation.

The ALS Safety Configuration Control (ASCC) software application was initially designed to track beamline statuses, key-enables, safety inspections, radiation surveys, and work authorizations. The software has expanded to include various schedules, ALS procedures, and reviews and is under continued development to manage annual tests and the beamline review process.

Annual Beamline Safety Day. A full evaluation of hazards at the beamlines is scheduled annually, one beamline at a time. User beamtime is suspended at that beamline in order to dedicate the time to

daylong safety-oriented activities. This day combines the annual beamline safety inspection, the annual beamline radiation surveys, and training on beamline radiation safety and beamline-specific ALS procedures. It involves beamline staff, floor operators, ALS safety management, and beamline line-management supervisors, as well as ALS and LBNL subject-matter experts. Issues that require correction or improvement are assigned and tracked with software. During the COVID-19 pandemic, much of the Safety Day activities were moved to a week-long safety effort to reduce crowding at the beamlines and to accommodate staff schedules during restrictions on employee headcount at the Laboratory.

Training. The ALS training program continues to grow with new courses. The ALS developed a COVID-19 course to describe how Lab safety protocols applied at the ALS. This course was active when the first waves of staff returned to the worksite. The required safety course for badge access, ALS1001, was overhauled to provide broad content, more interaction, and to target the various audiences who enter the ALS facility, including users, vendors, and emergency staff.

Continued user support. The ESAF, which is the online ISM evaluation form for users, is used to coordinate the work of all users, including users of beamlines supported by PRTs, to achieve floor-wide user coverage. Ongoing improvements have been made in the ESAF to enhance early communication between users and ALS safety staff. Online training is being developed to improve user understanding of the ESAF process.

Incorporation of ALS-U work into the ALS ISM process. Work for the preparation and installation of equipment needed for ALS-U must be carried out with regard to standard work authorization, ALS safety procedures, and without impacting the accelerator safety envelope and ALS operations. A work evaluation and permitting process has been developed between ALS and ALS-U staff to ensure that this is done in an efficient and safe manner.

3 Accelerator and instrumentation projects

3.1 Accelerator projects

This section enumerates and describes the accelerator projects planned for the next five years. The projects are divided into reliability and performance improvement categories, which are described in two separate subsections. Tables for each of the two categories provide the basic information at a glance, and details about the projects can be found in the text.

3.1.1 Reliability improvement projects

Table 1. Accelerator reliability projects.

Project title	Type of project	Expected completion	Notes
Replacement of the legacy linac modulators	AIP	Q2 FY21	Completed in Q2 2021
Upgrade of the low-level rf (LLRF) controls for the electron gun, linac, and booster	AIP	FY24	To be initiated in FY22–23
Equipment protection system (EPS) upgrade	OPS		To be initiated in FY22–23. Completion date depends on funds and resource availability.
Radiation safety system (RSS) upgrade	OPS		Being initiated. Completion date depends on fund and resource availability.
Online radiation-shielding configuration control Phase I, II and III	OPS	FY22–23	Phase-I and II completed; Phase-III funded and initiated
Storage ring HVAC and utilities upgrade	AIP	FY22	Initiated

AIP: accelerator improvement project; OPS: operations project

A number of projects in this category will be completed or initiated during the next five years. Particular attention and priority are being placed on those accelerator systems that will continue to operate beyond ALS-U. These include the present ALS injector chain (gun, linac, booster, and most of the electron-transfer lines), equipment protection systems (EPSs), radiation safety systems (RSSs), most of the utilities, and a number of beam diagnostic systems. Projects in this reliability category include the following:

Replacement of the legacy linac modulators. This was the first upgrade of the ALS injector subsystems. In FY21 Q2, the two 26-year-old units were replaced with state-of-the-art commercial devices.

Installation and commissioning of the units, initially planned for the July 2020 shutdown, were postponed to the January 2021 shutdown due to the restrictions and limitations imposed by the COVID-19 pandemic. The new modulators are now in operation.

Upgrade of the low-level rf (LLRF) and legacy controls for the electron gun, linac, and booster. This is the next main upgrade of one of the critical ALS injector sub-systems. New digital systems will replace the obsolete analog systems presently in operation. Such upgrades will improve reliability but also, and in a significant way, the overall performance and stability of the system. The project will be initiated in late FY22 or early FY23.

EPS upgrade. Each of the ALS sectors is equipped with an EPS system to protect front-end and beamline components during operation. The present system is fully operational, but it is based on obsolete components and on a not-fully-optimized architecture and distribution. The plan is to redesign the front-end systems to overcome these limitations and to gradually replace them sector by sector. The project will be initiated in FY22 and will continue in the years to come, with the completion date dependent on resources and funds availability.

RSS upgrade. Each of the ALS beamlines is equipped with an RSS system to protect personnel from radiation exposure during operation. The present system is fully operational but it is based on obsolete relay logic. The plan is to redesign the RSS systems using state-of-the-art programmable logic controller (PLC) technology and to gradually replace them. The project has been initiated by the development of a prototype system for one of the ALS beamlines and will continue in the years to come, with the completion date dependent on resources and funds availability.

Online radiation shielding configuration control. ALS beamlines use a complex and custom set of radiation shielding arrangements that require careful configuration control to avoid undesired personnel radiation exposure. The previous control system was based on a number of physical forms that needed to be filled out and linked together depending on the particular beamline at which the radiation shielding operation was being performed. Phase-I of this project, completed and in operation, moved the whole shielding configuration control system to a computer-based online application, effectively mitigating the risk of human errors while performing these critical operations. Phase-II, also completed and in operation, extended the configuration control to areas other than shielding, and Phase III, funded and initiated, will include the support and management of the activities related to the Accelerator Review Committee and of the Beamline Review Committee.

Storage ring HVAC and utilities upgrade. The present temperature-control system inside the ALS storage ring shielded area is obsolete and needs to be replaced. In addition, the existing system is located in a position that interferes with the installation of the accumulator—the new ring that will be added as part of the injector chain for the upgraded ALS—and needs to be relocated. The upgrade is being initiated and needs to be completed before the installation of the accumulator in FY22–23. Similarly, some of the utility systems need to be modified within the same time frame to allow for future operation of the upgraded ALS and of its subsystems.

3.1.2 Performance improvement projects

Table 2. Accelerator performance projects.

Project title	Type of project	Expected completion	Notes
ALS rf distribution system upgrade	AIP	FY22–23	Funded and initiated.
High-bandwidth kHz-class fast orbit feedback upgrade	AIP	FY21	Completed and in the fine tuning/optimization phase.
Fast EPICS-ready digitizer	OPS	FY22	Home-brewed digitizer to replace ZTEC digital oscilloscopes used along the facility. Funded, commissioned, and under deployment.
Development of next-generation beam position monitors (BPMs)	OPS	FY22–23	Approved.
Machine-learning applications for the ALS accelerator	OPS		First phase funded and initiated. Continuation after FY21 depends on fund availability.

AIP: accelerator improvement project; OPS: operations project

A number of accelerator projects targeting performance improvements to ultimately provide users with a better-quality photon beam are planned in the years preceding the ALS-U dark time. These projects will provide benefits and performance improvements to the present ALS and further enhance the performance of an upgraded ALS.

ALS rf distribution system upgrade. The numerous rf systems that allow the synchronized operation of the ALS facility accelerators (gun, linac, booster, and storage ring) receive their operating frequency from a single source represented by a high-stability, high-quality rf synthesizer. Downstream of that, the rf distribution system takes this master frequency and splits, down-converts, up-converts, and formats it to properly feed all the different “client” systems. The upgrade will replace the legacy components with state-of-the art technology counterparts to create a new setup fully integrated with the (recently upgraded) ALS high-performance timing system. The project has been initiated and will be completed in FY22–23. The upgraded rf distribution will provide much higher operational flexibility and performance stability to both the current and upgraded ALS.

High-bandwidth kHz-class fast orbit feedback upgrade. The present ALS is equipped with two feedback systems to maintain beamline source points fixed with micron/submicron precision. One of the feedbacks, the slow orbit feedback, compensates for slow beam orbit drifts, mostly driven by thermal cycles (day/night, seasonal, etc.). The second system, the fast orbit feedback, is designed to mitigate the effects of faster variations. The present ALS fast orbit feedback has a bandwidth limited to about 60 Hz. A project to upgrade the fast feedback to a kHz-class bandwidth was funded and initiated. The activities are structured in three main parts: upgrading the ALS BPMs and their cell controllers to digital high-performing electronics (this part was completed in FY20); replacement of corrector power supplies with

high-bandwidth components (48 new fast power supplies have been procured and installed in FY20); replacement of 22 aluminum vacuum-chamber spool pieces (located inside the corrector magnets) with stainless-steel counterparts to reduce eddy-current attenuation of high-frequency (kHz) magnetic fields (this part is in an advanced state and was recently completed in FY21). The system is now in its final fine-tuning/optimization phase. A similar system architecture will be used in the upgraded ALS.

Fast EPICS-ready digitizer. The operation of an accelerator facility like the ALS requires the monitoring of a large number of pulsed signals coming from different accelerator subsystems. This requires the use of high-performance digital oscilloscopes fully integrated into the accelerator control system. The presently used scopes are now obsolete and starting to show signs of reduced reliability. To replace them, a project for the development of state-of-the-art, high-bandwidth, fast digitizers has been funded and initiated. The new units allow for direct integration into the ALS control system, based on EPICS. Two prototypes, fabricated in FY19 and FY20, demonstrated the required performance. Production of the final operational units was completed in FY21, and the deployment of the units at the ALS will continue in FY22.

Development of next-generation beam position monitors (BPMs). The position stability of the electron beam in the storage ring directly affects the stability of the photon beam and the spatial resolution of the beamlines. The pursuit of higher and higher spatial resolutions requires an electron-beam stability beyond presently achieved performance. Higher-resolution beam position monitors (BPMs) for electrons are necessary for next-generation diffraction-limited storage rings such as the planned upgraded ALS. In such rings, the electron and photon beam sizes dramatically decrease, requiring the development of higher-resolution BPM electronics. A project for the development of prototype BPMs with a performance that matches the needs of the upgraded ALS has been approved. Completion and testing of such prototypes are expected in FY23.

Machine-learning applications for the ALS accelerator. ML techniques are finding applications in nearly every field of human activity, including particle accelerators. At the ALS, a new activity was initiated in FY19 to develop ML accelerator applications to control and improve the performance of the ALS. The project, funded by the DOE Accelerator and Detector Research program (ADRP) of the Basic Energy Sciences program, and the DOE Advanced Computing Science Research (ASCR) program, successfully developed a new scheme using deep-learning techniques to effectively compensate for beam-size variations induced by insertion devices. Additional details can be found in section 3.5.2 of this document. The second phase of this activity is now targeting the development of ML-assisted, multi-objective optimization using genetic algorithms (MOGA). Initial results are already showing that the synergetic use of ML and MOGA can reduce optimization times in complex multi-variable, multi-objective problems by orders of magnitude. Funds for this activity will presently terminate in FY21, but continuation funds for these very promising activities are being pursued.

3.2 Photon-science projects

3.2.1 Beamline instrumentation projects under construction or in commissioning

Table 3. Photon-science projects currently in commissioning (green) and design, procurement, construction (blue).

Source point	Project title	Target commissioning	Partner and funding	Scope and notes
7.0.1.1	COSMIC scattering	Continuing	DOE midscale, ALS EQU	Half-length undulator and SXR beamline for XPCS studies of spontaneous fluctuations in spin, quantum, and topological materials
2.0	GEMINI	Continuing	HHMI, LBNL/MBIB	In-vacuum undulator monochromator; microfocus optics for macromolecular crystallography; advanced detectors; robotic sample handling
6.0.1	AMBER	Continuing	PNNL, JCAP, JCESR, ALS EQU	Repurpose undulator; multimodal SXR in situ/operando spectroscopy studies of catalysis, earth & environment, and energy conversion
6.0.1	AMBER-2	Start 2022	ALS EQU	Second branch for high-throughput spectroscopy
6.0.2	QERLIN	Start 2022	Moore Foundation, ALS EQU	Repurpose undulator; soft x-ray RIXS beamline & double-dispersion design for high throughput & resolution; spin & quantum materials
4.0.3	MERLIN upgrade	Long-lead procurement placed	ALS EQU	High-energy-resolution beamline for ARPES and spin-resolved ARPES

ALS EQU: ALS equipment funding; XPS: x-ray photoelectron spectroscopy; SXR: soft x-ray; BL: beamline; ES: endstation

Table 3 summarizes ALS beamline and endstation projects with a total cost over \$0.5M presently being commissioned or under development. The first three projects are in commissioning. Two additional beamline projects will finish construction in 2022, and the commissioning of the beamlines and endstations will start soon after. The upgrade of 4.0.3 is at an earlier design and procurement stage and is currently on hold.

COSMIC (now). Since 1995, the ALS has led the world in developing soft x-ray (SXR) STXMs. One branch of COSMIC is optimized for ptychographic diffractive imaging with state-of-the-art scanning systems, high-data-rate charge-coupled device (CCD) detectors matched to a high-bandwidth data system, and diverse in situ sample environments and is available to users. COSMIC provides images with <5 nm resolution, combining 3D tomographic reconstruction with full chemical contrast. A second branch of the COSMIC beamline and associated endstation is devoted to probing spatial correlations in spin and quantum materials in the time domain by enabling SXR XPCS and various speckle metrology experiments, and commissioning of the endstation is continuing.

Gemini beamline (now). The macromolecular crystallography beamlines at the ALS have enabled outstanding scientific productivity, providing high-performance hard x-ray diffraction capabilities that have kept pace with the changing needs of the structural biology community. To continue to provide the highest possible performance, HHMI has funded a new high-brightness protein crystallography facility called Gemini in ALS Sector 2. A high-brightness, in-vacuum undulator beamline has been installed, and the commissioning of the beamline and endstation is continuing. The beamline is designed to eventually serve two branchlines, located in a single hutch, simultaneously. One of the branches will be served with diamond beam-splitters and operate at fixed wavelength; the other will allow variable-wavelength operation for multi-wavelength anomalous dispersion measurements.

AMBER and AMBER-2 (now and 2022). AMBER was enabled by the repurposing of Sector 6. The beamline is optimized for advanced-materials preparation and multimodal, high-throughput, operando analysis of chemical and energy systems, thereby improving ALS capabilities and increasing capacity in this area. AMBER will provide in situ sample preparation with RIXS and XAS spectroscopies. AMBER is developed in partnership with Pacific Northwest National Laboratory (PNNL) and the Joint Center for Artificial Photosynthesis (JCAP) and the Joint Center for Energy Storage Research (JCESR) Energy Innovation Hubs. Construction of the first branch was completed in 2020 and commissioning has started. Work has started on a second branch, which will broaden the technical capability of the beamline for high-throughput operando RIXS.

QERLIN (2022). A strength of ARPES is that it measures the coupling of electrons and holes to low-energy excitations. However, it can be difficult to identify which excitation(s) lead to a particular emergent property. It is crucial to measure the dispersion relations of the low-energy excitations directly, with high resolution, with SXR contrast, through crucial regions of the phase diagram, and over a large region of Fourier space. For this reason, one of the highest ALS priorities is to build and commission a new SXR RIXS beamline called QERLIN. The QERLIN beamline is enabled by the repurposing of Sector 6 following decommissioning of the ultrafast slicing sources, and is based on a novel optical design that involves multiplexing the incident beam across the face of the sample and the scattered beam across a high-resolution pixelated detector. This will provide a resolving power of >10,000 and will probe an entire map of photon energy in vs photon energy out in parallel—a 100-fold increase in throughput. Major components of the beamline have been installed, and construction of the endstation and the spectrograph is continuing. Commissioning will start in 2022.

ALS Beamline 4.0.3 upgrade. The design and procurement of improved optics for the MERLIN beamline was completed and several components, including a new monochromator, have been ordered. The upgrade will significantly improve the performance of the beamline in regard to energy resolution, flux, and stability and will prepare the beamline for new ARPES methodologies that require high brightness, flux, and energy resolution, e.g., ultrahigh-energy-resolution spectroscopy, spin-resolved ARPES, and momentum microscopy. This upgrade will ready the beamline for ALS-U.

3.2.2 New ALS-U and ALS beamline projects

Table 4. ALS-U (blue) and ALS (gold) beamline (by location) and endstation (ES) projects prioritized for development.

Source point	Project title	Target commissioning	Partners & funding	Scope and notes
8.0.1	Tender x-ray beamline	After ALS-U dark time	ALS-U	Beamline for tender-energy coherent scattering and microscopy
10.0.1	FLEXON beamline	After ALS-U dark time	ALS-U	Beamline for soft x-ray photon correlation spectroscopy and nanofocus elastic and inelastic scattering
7.0.1	COSMIC upgrade	After ALS-U dark time	ALS-U	Beamline for soft x-ray microscopy, ptychography, tomography
7.0.2	MAESTRO upgrade	After ALS-U dark time	ALS-U	Beamline for nano-scale ARPES
4.0.2	Magnetic spectroscopy & microscopy	TBD	ALS	Reliability and brightness upgrade of beamline for spectroscopy, microscopy and resonant scattering
ES	Low-T SINS	TBD	ALS	Low-temperature and nanometer-resolved infrared spectroscopy setup for quantum materials research

Table 4 contains a new set of projects selected for development by the ALS and also through ALS-U. The table includes four prioritized ALS-U project beamlines and two proposed ALS beamline upgrades. The planning process for ALS-U and ALS beamlines was informed by several workshops organized by ALS-U and the ALS and by five crosscutting reviews in 2017–2018 that reviewed ALS beamlines. To maximize the scientific impact of the ALS upgrade, a synergistic strategic plan for ALS and ALS-U beamlines was developed during the last year, and all new beamlines will be designed to make use of the improved performance of the ring after the upgrade.

The ALS-U beamlines were selected in an ALS-U-supervised beamline selection process. A working group of LBNL scientists created 15 initial beamline proposals based on reports from a series of workshops attended by synchrotron radiation scientists and ALS users. The output of these workshops is documented in the report, “Solving Scientific Challenges with Coherent Soft X-Rays.” A down-select process guided by an LBNL internal steering committee and advised by an ALS external ad hoc committee with participation from the ALS scientific advisory and ALS-U technical advisory committees created a final set of scenarios from which the ALS-U Project selected the final list of project beamlines. To receive broad input and communicate progress in the beamline selection process, ALS and ALS-U organized user forums hosted by the ALS UEC and solicited input and feedback from the user community. Updates about the status of the selection process were given at the ALS User Meeting and at advisory committee meetings.

The ALS-U Project plans to build two new beamlines—a soft x-ray beamline in Sector 10 dubbed “FLEXON” (FLuctuation and EXcitation of Orders in the Nanoscale) and a tender x-ray beamline in Sector 8. It will also upgrade two existing soft x-ray beamlines in Sector 7, COSMIC and MAESTRO (Microscopic And Electronic STRucture Observatory). The ALS has prioritized the upgrade of Beamline 4.0.2, a beamline for magnetic spectroscopy and scattering that will be ready to utilize the 100 times greater brightness of the ALS after the upgrade, and is preparing for an upgrade of the second beamline in this Sector, Beamline 4.0.3.

ALS-U FLEXON beamline. Sector 10 will house the FLEXON beamline, a high-brightness coherent soft x-ray beamline for probing the roles of multiscale heterogeneity in quantum materials. FLEXON will integrate multiple complementary techniques to provide multimodal probes required for revolutionary progress in understanding the complex physics of quantum materials. One branch will be optimized for high efficiency and medium energy resolution for XPCS and nano-RSoXS. The second branch will provide x-rays with high energy resolution in a nanofocused spot and will be optimized for coherence-requiring imaging techniques. XPCS experiments will achieve an improvement in time resolution of three to four orders of magnitude over the current ALS, while diffraction imaging techniques will enable measurements with up to 10-fold improved spatial resolution.

ALS-U tender x-ray beamline. Sector 8 will house a new tender x-ray beamline designed to address challenges at the frontiers of diverse scientific areas, ranging from soft condensed matter and biomaterials to energy science and earth/environmental science. One branch will feature coherent scattering capabilities enabling operando and in situ studies of materials in the tender energy range. The second branch will be optimized for STXM. The brightness of the upgraded ALS in this energy range, when coupled with advanced detectors and experimental systems, will allow for coherent x-ray scattering with microsecond time resolution and scanning spectromicroscopy with spatial resolution of a few nanometers.

ALS-U COSMIC upgrade. The ALS-U Project upgrade of COSMIC will consolidate the ALS’s insertion-device STXM instruments (currently occupying 7.0.1.2 and 11.0.2.2) on a single straight section. Following the upgrade of the beamline optics, the full brightness of the upgraded ALS will be available for zone-plate-based microscopy, ptychography, and 3D tomography, all of which require coherent illumination of the zone plate and the sample. The upgrade will lead to an up to 100-fold increase in measurement speed and an improvement in spatial resolution down to 1 nm.

ALS-U MAESTRO upgrade. The MAESTRO beamline makes use of zone-plate and reflective focusing optics to investigate the electronic, chemical, and morphological structure of in situ deposited materials using scanning probe and full-field ARPES instrumentation. The upgrade will improve the ARPES collection efficiency by more than an order of magnitude.

ALS Beamline 4.0.2 upgrade. This proposed ALS beamline upgrade will renew the optics of the beamline, which serves the magnetism and quantum materials community. The monochromator will be replaced with a state-of-the-art-system, and some mirror systems will be upgraded with brightness-preserving optics compatible with ALS-U. The ALS Photon Science Development team has developed a design package that will be executed when funding and resources have been identified.

Low-T SINS. The ALS is preparing to develop a cryogenic endstation for broadband infrared nanospectroscopy in the far-IR in a UHV environment that will enable exploration of new nanoscale

physics in novel materials near phase transitions. SINS combines the high brightness, broad spectral bandwidth, and spatial coherence of synchrotron infrared radiation with the high spatial resolution and sensitivity of scattering-type, scanning near-field optical microscopy (s-SNOM) to achieve broadband infrared spectroscopy with nanometer spatial resolution.

While the ALS continues to innovate new and to upgrade existing experimental systems, the facility carefully balances its suite of instruments with the staff it is able to support so as to maintain efficient and sustainable operations. The design, commissioning, and operation of most of the projects listed above will be handled by existing ALS scientific staff who have been managing the beamlines and instruments being upgraded, or in some cases being shut down. Overall, these projects are intended to be net staffing neutral.

3.3 Detector development

The ALS Detector Development Program focuses on the development of novel soft x-ray detectors that enhance the productivity of the ALS and enhance the facility's scientific reach. The program is also involved in efforts to help plan and optimize detector capabilities for the upgraded ALS. Soft x-ray detection has challenges not present in hard x-ray detection: signal-to-noise issues (with one-tenth the energy of hard x-rays), in-vacuum operation, and detection efficiency (shallow penetration of soft x-rays into a detector). Several of the techniques and beamlines described above (ptychography, STXM, COSMIC, QERLIN, etc.) are enabled by detectors developed by this program.

The FastCCD, developed in collaboration with the detector group at the Advanced Photon Source (APS), is now deployed at the ALS, APS, Linac Coherent Light Source (LCLS), National Synchrotron Light Source II (NSLS-II), and the European X-Ray Free-Electron Laser Facility (XFEL). It is used for scanning microscopies at the ALS, and several new deployments at ALS beamlines are planned. The VeryFastCCD, the next generation of the FastCCD, is being developed in a collaboration with SLAC National Accelerator Laboratory (SLAC) as an LCLS-II soft x-ray detector and will be an obvious upgrade for scanning microscopies at the ALS as brightness increases. Testing of this detector at the ALS is underway, and we expect deployment on ptychographic microscopes shortly.

The SpectroCCD, a very-fine-pitch ($5 \times 45 \mu\text{m}^2$) detector for (1D) RIXS, has proven key to obtaining the resolution needed for momentum-resolved RIXS (qRIXS). The detector has been commercialized through the DOE Small-Business Technology Transfer (STTR) program and is now in routine use on the qRIXS endstation at Beamline 8.0.1. QERLIN presents the challenge of high spatial resolution for 2D RIXS, at a comparatively high rate. Here, the group has leveraged its experience in pioneering CMOS (complementary metal-oxide semiconductor) detectors for electron microscopy to develop a $5 \times 5 \mu\text{m}^2$ soft x-ray, high-rate CMOS detector.

Future soft x-ray detector advances will be needed to cope with the higher rates provided by improvements in optics and sources, notably due to ALS-U. For example, we are actively collaborating with the University of California (UC) Space Sciences Laboratory to investigate and develop hybrid detectors that combine channel plate sensors that feed pixelated CMOS TimePix detectors for several of these applications—fast XPCS, time-resolved spectroscopy, and high-resolution RIXS. Initial testing of the TimePix2 detector already has produced promising results. The next-generation TimePix3 detector under development will enable full-speed readout of the entire array.

Workshops every one to two years at ALS User Meetings and elsewhere are forums to collect community need and interest, and, together with the Photon Science Group, drive our priorities. ALS operating funds are used to deploy the detectors we develop and to adapt them to specific experiments and beamlines.

3.4 X-ray optics and metrology

This section describes the tools and techniques that are being developed to enable the construction of a new generation of beamlines and endstations, as outlined in section 3.2. One of the challenges will be to cope with beam sizes in the horizontal direction that are 30 times smaller than the beams we have today. This requires horizontally focusing mirrors to be of much higher quality, and to have a surface figure under load that deviates from the theoretically perfect figure by less than 1 nm. The absorbed power load is typically a few hundred watts. Such tolerances require large improvements in fabrication quality and in mirror cooling technology. Fortunately over the last decade, major advances in fabrication have been made, and even fairly complex figures can now be made to the requisite tolerance. Significant advances, though, are required in mirror cooling, and this is an area of active research.

The major challenges relate to cooling and suppression of vibration. High-power mirrors at the ALS traditionally have used an internally cooled copper structure. Calculations show that at the new tolerance levels we need, this basic structure is inadequate. This type of structure will be replaced by highly optimized water-cooled silicon mirrors, or silicon mirrors cooled by liquid nitrogen to around 124 K, the point at which the expansion coefficient becomes zero. Both routes require significant R&D to prove the technology before deployment in beamlines. Not only do the high-power mirrors in high-brightness beamlines have to be upgraded, all horizontally focusing mirrors in these beamlines need mirrors built to this new tolerance.

In addition to manufacturing and thermal tolerances, vibration becomes a major factor in the performance of a beamline at this tolerance level. One area of work is centered on reduction of cooling-fluid-induced vibration by performing R&D on the modeling of turbulence in cooled systems, the use of optimum geometry and diffuser structures to reduce vibration, and the implementation of stiffer support mechanisms. Part of this ongoing work is to survey the vibration we currently have on the ALS floor and in some of our insertion-device beamlines.

Another area of concern is the slow drift of optics due primarily to ground motion and relaxation of support mechanisms. For regular alignment of the beamline, we intend to use multilayer imaging devices that can be inserted into the beamline; this will allow us to find the beam center, and together with electron BPMs, the beam angle. A combination of this type of device and photodiode and photoemission monitors will allow us to track the position down the beamline. Unlike present-day ALS beamlines, each component will be movable using motor-controlled systems. The combination should allow us to do routine realignment of the beamlines in a simple way, compared to the manual methods we use today.

All of the techniques outlined above most probably will not be sufficient to ensure preservation of the beam brightness and reduction of noise and drift to the required levels. To go beyond this, we are developing wavefront sensing and adaptive wavefront control. The wavefront sensing uses grating-based interferometry, and feedback will be used to adjust pre-figured mirrors that have integral piezo

systems to create high-order corrections to the surface height. The aim is for these systems together to work with a bandwidth of >150 Hz, i.e., to a regime where mechanical vibrations are small.

The result of this work should be a new toolbox of techniques in mirror cooling, mounting, alignment, stabilization, and beam monitoring that should significantly improve the quality of beam that is delivered to users.

An integral component of the optics program at the ALS is the X-Ray Optics Laboratory (XROL). This group assures the quality of the optical components installed in beamlines or used in endstations. For example, we must ensure that the mounting system of mirrors does not cause undue deformation in operation, and that the system under adjustment or water flow has the desired characteristics. The XROL delivers the state-of-the-art optical metrology required to build and maintain high-performance operation of ALS beamlines. For example, the upgraded Long Trace Profiler (LTP-II) and Developmental Long Trace Profiler (DLTP) are capable of 1D surface-slope profiling with a proven accuracy of tangential slope measurements with flat optics of about 60 nrad (rms) and with significantly curved optics (radius of curvature of ≥ 15 m) of around 200 nrad, limited by the profiler's systematic errors. The increasing brightness of ALS is driving our program to even higher measurement accuracy. For next-generation optics, we need an absolute slope accuracy of 50 nrad and a height accuracy of <0.5 nm in many cases. In close collaboration with optics teams from other DOE BES facilities as well as with our colleagues around the world, we are developing new methods that should take us to these goals within a few years.

Specific optical metrology challenges to be addressed are the development of the required ultrahigh-accuracy x-ray mirror and diffraction-grating characterization instruments. Major XROL efforts will be directed to R&D on a new optical surface measuring system (OSMS) capable of 2D surface-slope metrology with an accuracy below 50 nrad (absolute). Another promising technique is stitching interferometry, similar to the MSI/RADSI (microstitching interferometry/relative-angle determinable stitching interferometry) system recently developed at the Ultra-Precision Machining Laboratory at Osaka University.

A third component of our work is to develop unique optical elements, where required by the ALS experimental program. For example, we require diffraction gratings with very high efficiency and resolution for RIXS. Maximizing efficiency requires the use of multilayer coatings, which in turn require the grating facets to be atomically smooth. We have developed this technology, and it will be deployed for the first time in the high-resolution QERLIN RIXS spectrometer. Another example is the development of “diaboloid” optics for bending-magnet beamlines, which can take a cylindrical wave and focus it to a point focus. R&D is being done on the fabrication of these optics using modification of the surface using a varied-thickness coating.

3.5 Data management and computing

The Light Source Data and Computing Steering Committee (LSDCSC), composed of members from the five BES light sources, has evaluated and quantified the long-term needs for data analysis, management, and storage across the five BES light sources. The estimates present a daunting challenge: in 10 years, the LSDCSC estimated that, collectively, these facilities will produce up to 1 exabyte (quintillion bytes) of data per year and will require a peak on-demand computing resources of 1 exaflop (quadrillion floating-

point operations per second). The ALS alone is estimated to require much less than this—a mere 210 petabytes (quadrillion bytes) per year and 30 petaFLOPS during peak, numbers that even by themselves will require serious effort to achieve.

The LSDCSC outlined computing challenges in four main areas:

- Data-management and workflow tools that integrate beamline instruments with computing and storage resources, for use during experiments, as well as facile user access for post-experiment analysis.
- Real-time data analysis capabilities to significantly reduce data volumes and provide feedback during experiments to improve data quality and to drive the direction of ongoing measurements.
- On-demand utilization of supercomputing environments to enable real-time data processing.
- Data-storage and archival resources to house the continually increasing amounts of valuable scientific data produced by the BES light sources.

With challenge comes opportunity, and the ALS is enthusiastic about pursuing these opportunities. The challenges bulleted above are endemic to light sources and other kinds of facilities around the world, and it makes sense to collaborate to find cross-facility solutions. Recently, BES management encouraged such a collaboration among the BES light sources and also defined a structure to find solutions. This collaboration will necessarily include ASCR-supported high-performance computing and networking facilities and, as importantly, the expertise of their respective staffs.

To address the approaching data challenges, the ALS is developing data-driven acquisition solutions, data workflows for near-real-time analysis, web-based graphical user interfaces for analysis, advanced data transfer solutions to large storage and compute facilities and soon seamlessly coupled with integrated ML solutions. These emerging capabilities are described in more detail below.

3.5.1 Data management tools

The ALS Computing Program, together with beamline scientists and users, is developing data management tools that assist users and staff during the full data lifecycle from acquisition to storage and analysis. These tools include software that runs at the beamline to detect, package, and transfer new data; database servers that register data with its associated metadata to allow subsequent search and organization; and workers, message-passing systems, and workflow tools that allow automated processing to be launched on data sets using local and remote resources (such as supercomputing centers) as data arrives. Stored metadata will cover information about experiments, the beamline environment, and pointers to raw and derived data that is stored in a variety of locations. An easy-to-use web portal will allow users to view or download results during or after their beamtime. The web portal also allows users to seamlessly move their data into the Jupyter environment for further processing.

Table 5. List of data management, analysis, and workflow tools currently under development.

Tools	Description
Implementation of Bluesky	The ALS is developing procedures for beamline automation and simplification of common tasks and is integrating the Bluesky (NSLS-II) toolchain in a data acquisition graphical user interface that will execute complex acquisition “plans” through simple button clicks.
Graphical User Interface Xi-CAM and web solutions using dash/plotly	ALS and CAMERA are developing this Python and Qt-based graphical user interface as an integrated platform for synchrotron data acquisition, management, visualization, and analysis. The program plans to: a) add scripting tools to pre-existing LabView controls, b) enable parameterized analysis using metadata from Databroker databases, c) enable exploratory analysis using interactive visualization tools, and d) support workflow-driven data processing powered by Dask. The ALS Computing Program is currently in the process of replacing the software with a more web-based solution to address the need for remote data access and processing.
Implementation of CAM-Link data processing workflows	CAM-Link, developed by the ALS and CAMERA, will support data movement and execution workflows across one or more facilities. CAM-Link will provide: a) an automatable process for authentication and authorization enabling distributed end-to-end pipelines, b) interfaces for analysis routines communicating across multiple facilities, c) resource provisioning support for backend resources such as remote job schedulers, d) interfaces for moving data and extracting metadata information, and e) tools enabling the execution of analysis workflows and real-time feedback.
Networking and computing infrastructure	The ALS will design a reference architecture for beamline networking and computing hardware utilizing existing ALS network, LBLnet, and ESnet structures while taking advantage of the ScienceDMZ model.
Experiment metadata database	The ALS is designing a metadata repository and accompanying web portal to store metadata about user experiments. The system will coordinate with various metadata capture tools (sample data, electronic notebook, etc.) to gather information about experiments, which can be reviewed later. The ALS is using a software called SciCAT, which is developed by multiple synchrotrons across Europe.
RAC	RAC is a new tool that enables secure remote access to ALS beamline computers via a portal that is embedded in ALSHub.
Jupyter hub environments	The ALS is currently developing a solution to connect jupyterhub directly to SciCAT with the single click of a button. On top of Jupyter, several graphical user interfaces have been developed.

3.5.2 Machine learning

ML concepts provide a novel and transformative mechanism to develop powerful real-time processing solutions for large and complex data sets. Applications at the ALS range from improving the electron beam stability, which all users will benefit from, to assisting and guiding scientific discovery at individual beamlines.

The ALS is developing a collaborative ML platform for scientific discovery in collaboration with other BES light sources and nanoscience centers and participates in projects funded by the 2020 DOE call for “Data, Artificial Intelligence, and Machine Learning at DOE Scientific User Facilities (MLExchange).” Led by the ALS, a set of tools is being developed to make ML architectures and models available to users and facility scientists. One of the milestones is to develop a user-friendly interface to manually or automatically label data that can then be fed into ML models to speed up data analysis and materials characterization. A layout of the MLExchange architecture can be seen in Fig. 10.

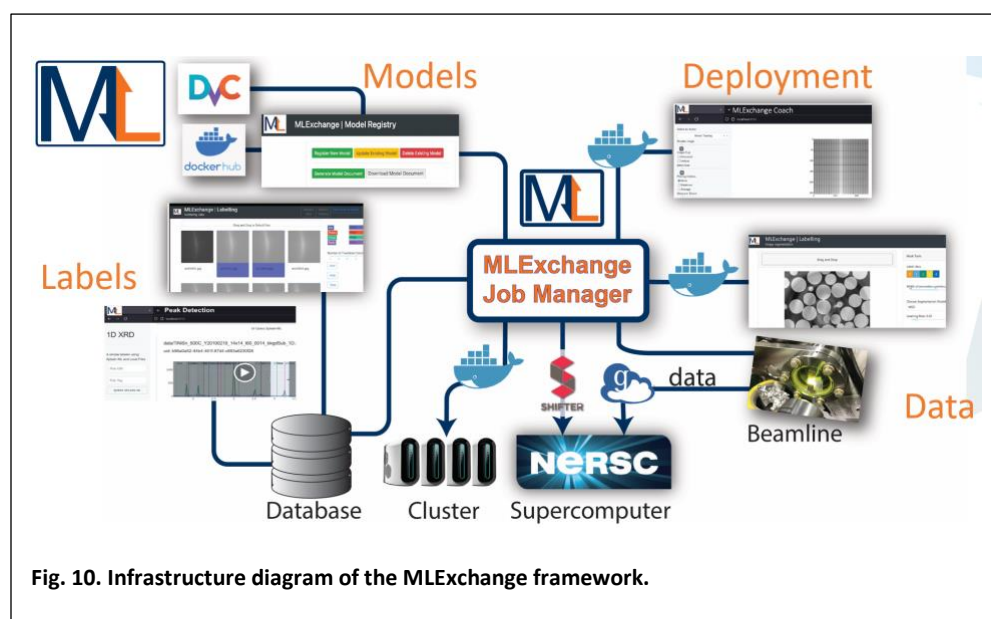


Table 6. List of machine-learning-enabled software tools currently under development.

Tools	Description
Electron beam size stabilization	The ALS has developed a ML model based on a complete set of metadata from the storage ring and implementing a neural-network-based correction loop. Vertical beam variations have decreased by an order of magnitude since the ML-enabled loop is operating.
Pattern recognition for images and volumes	ALS and CAMERA are developing ML based tools to extract quantitative information from acquired 2D and 3D data. ML tools aid users in transitioning to more autonomous modes of data analysis, e.g., providing tools for feature extraction, detection, segmentation, and classification at beamlines acquiring image and volumetric data.
Pattern recognition of scattering patterns	ALS and CAMERA are developing convolutional neural network tools to aid the high-throughput analysis of x-ray scattering data. A trained model successfully recognized grazing-incidence small-angle x-ray scattering patterns with a rate of 98% from simulated data.
ML platform for scientific discovery	Research and develop the construction of new mechanisms for data labeling and to automatically extract features.

4 Initiatives and emerging beamline and endstation development opportunities

Guided by the TA priorities discussed in section 2.1, the ALS seeks to develop new beamline instrumentation over a time window of five to ten years, which will significantly enhance our existing capabilities in synchrotron science. These proposed instrumentation upgrades have been endorsed by ALS crosscutting reviews and workshops and have strong user community support. The ALS is seeking partners to support and realize these initiatives, which target important growth areas in x-ray science at the ALS. The ALS intends to prioritize and execute projects from this list as resources become available.

Table 7. Emerging beamline and endstation development opportunities (not in any order of priority).

Source point	Project title	Scope and notes
9.3.2 or 9.1.1	APXPS bending-magnet beamline	Bending-magnet beamline optimized for soft-x-ray ambient-pressure photoemission spectroscopy, upgrading or replacing 9.3.2
11.0.2	11.0.2 upgrade	Upgrade of beamline to go into the tender x-ray regime for operando APXPS/Scattering/RIXS interfacial science
TBD	SAXS/WAXS	High-throughput scattering beamline at an ALS-U high-field port
Endstation	SPIN-MM	Low-temperature, high-resolution ARPES and momentum microscopy instrument at BL 4.0.3
Endstation	Q-STXM	STXM endstation optimized for high-field, low-temperature magnetic microscopy at BL 4.0.2
Endstation	Tender STXM	Tender nanoprobe endstation with a spatial resolution of a few nm to enable operando multimodal microscopy at ALS-U BL 8
Endstation	Tender Scattering	Scattering endstation to study spatio-temporal behavior/XPCS of soft matter/bio/energy materials at ALS-U BL 8
Endstation	Coherent Scattering	Coherent scattering endstation (XPCS) for quantum materials at ALS-U BL 10 (FLEXON branch 1)
Endstation	Novel Imaging	Novel imaging endstation using coherent light for quantum materials at ALS-U BL 10 (FLEXON branch 2)

Beamline 9.3.2 APXPS replacement. Beamline 9.3.2 serves a strongly growing community utilizing soft x-rays to study surface catalytic reactions and electrochemistry using x-ray photoelectron spectroscopy at ambient pressures, a priority of the Chemical Transformations TA. The obsolete beamline optics need to be updated by building a replacement beamline at port 9.3.2 or at 9.1.1. Plans are being developed for a possible start after the ALS-U dark time.

Beamline 11.0.2 upgrade. This high-brightness beamline initiative is a priority of the Chemical Transformations TA. The upgraded beamline targets a combination of RIXS and APXPS, in an operando environment and paired with coherent scattering and nanofocusing. The upgrade would offer tools to

study interfacial chemical reactions dynamically in liquid jets and at surfaces with down-to-nanoscale spatial resolution and down-to-microsecond temporal resolution. Initial R&D has been conducted through an LDRD.

Beamline 7.3.3 relocation. The ALS is seeking to relocate the SAXS/WAXS beamline from a warm-bend to an ALS-U high-field bending magnet, significantly increasing the performance and enabling high-throughput experiments for the soft-matter, bio, energy, and functional materials community.

Ultralow-temperature spin-momentum microscopy. The ALS seeks to develop new endstations for electronic structure measurements at very low temperatures below 1 K and in combination with efficient spin detection, a priority of the QMRD TA. One of the anticipated endstations would be a spin-momentum microscope, a high-throughput setup for momentum-, energy-, spin-, and position-dependent photoemission spectroscopy. The second endstation would have an optimized sample environment and spectrometer for ultrahigh-resolution electron spectroscopy at very low temperatures to map the electronic structure of novel exotic phases.

Q-STXM endstation. This low-temperature high-field STXM would be optimized for studies of the electronic, chemical, and magnetic properties of spin systems exhibiting nanoscale phases and would serve the magnetism, spintronics, and quantum materials community. This endstation is a priority of the QMRD and the CMI TAs. An LDRD proposal has funded successful exploratory work.

Tender x-ray endstations for ALS-U. The ALS seeks to develop two endstations that will be located at a beamline employing a full-length insertion device optimized for coherent, tender x-rays. These endstations will substantially enhance the ALS portfolio by accessing absorption edges such as Na, Ca, P, S, Si, and Ti that are relevant for biology and earth sciences, and by enabling studies of thicker samples due to the enhanced photon energies. One endstation would employ a nanoprobe operating in a STXM/ptychography mode for nanometer-scale spatial imaging, while the second would probe spatio-temporal dynamics using XPCS.

Soft x-ray endstations for ALS-U. The ALS intends to develop two endstations that will be located at a beamline employing a full-length insertion device optimized for coherent, soft x-rays. These endstations would allow access to higher spatial resolutions and shorter time scales than are currently accessible at ALS and are a priority of the QMRD TA. One endstation would focus on spatio-temporal dynamics using XPCS, while the other would employ novel scattering geometries and detection schemes for ultrahigh spatial resolution imaging of novel electronic and ordered phases.

5 List of abbreviations

ADRP	Accelerator and Detector Research Program
AI	artificial intelligence
AIP	accelerator improvement project
ALARA	as low as reasonably achievable
ALS	Advanced Light Source
ALS EQU	ALS equipment funding
ALS-U	Advanced Light Source Upgrade Project
AMBER	Advanced Materials Beamline for Energy Research
AP	Approved Program
APS	Advanced Photon Source
APXPS	ambient-pressure x-ray photoelectron spectroscopy
ARPES	angle-resolved photoemission spectroscopy
ASCC	ALS Safety Configuration Control
ASCR	Advanced Scientific Computing Research
BCSB	Berkeley Center for Structural Biology
BES	Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
BL	beamline
BPM	beam-position monitor
BSISB	Berkeley Synchrotron Infrared Structural Biology
CAMERA	Center for Advanced Mathematics for Energy Research Applications
CCD	charge-coupled device
CD	Critical Decision
CMI	Complex Materials and Interfaces
CMOS	complementary metal-oxide semiconductor
COMPRES	Consortium for Materials Properties Research in Earth Sciences
COSMIC	COherent Scattering and MICroscopy
CT	computed tomography
CXRO	Center for X-Ray Optics
DEI	diversity, equity, and inclusion
DFT	density functional theory
DLTP	Developmental Long Trace Profiler
DOE	Department of Energy
DT	digital twin
DWG	Data Working Group
EPICS	Experimental Physics and Industrial Control System
EPS	equipment protection system
ES	endstation
ESAF	Experiment Safety Assessment Form

FAIR	findable, accessible, interoperable, reusable
FAST	fast x-ray absorption spectroscopy in transmission
FLEXON	FLuctuation and EXcitation of Orders in the Nanoscale
FLOPS	floating-point operations per second
GISAXS	grazing-incidence small-angle x-ray scattering
GU	General User
HAXPES	hard x-ray photoelectron spectroscopy
HHMI	Howard Hughes Medical Institute
HVAC	heating, ventilation, and air conditioning
IDEA	inclusion, diversity, equity, and accountability
IR	infrared
ISM	Integrated Safety Management
IT	information technology
JBEI	Joint BioEnergy Institute
JCAP	Joint Center for Artificial Photosynthesis
JCESR	Joint Center for Energy Storage Research
JGI	Joint Genome Institute
LBNL	Lawrence Berkeley National Laboratory
LCLS	Linac Coherent Light Source
LDRD	Laboratory Directed Research and Development
LLRF	low-level rf
LSDCSC	Light Source Data and Computing Steering Committee
LTP	Long Trace Profiler
MAESTRO	Microscopic And Electronic STRucture Observatory
MBA	multibend achromat
MBIB	Molecular Biophysics and Integrated Bioimaging
MESB-U	Molecular Environmental Science Beamline-Upgrade
ML	machine learning
MOGA	multi-objective optimization using genetic algorithms
mRIXS	mapping of resonant inelastic x-ray scattering
MSI	microstitching interferometry
MX	macromolecular crystallography
NASA	National Aeronautics and Space Administration
NAWI	National Alliance for Water Innovation
NERSC	National Energy Research Scientific Computing Center
NLK	nonlinear kicker
NN	neural network
NSF	National Science Foundation
NSLS-II	National Synchrotron Light Source II
OPS	operations project
OSMS	Optical Surface Measuring System

pBPM	photon beam-position monitor
PEEM	photoemission electron microscopy
PLC	programmable logic controller
PNNL	Pacific Northwest National Laboratory
PRT	Participating Research Team
PS-D	Photon Science Development (branch of the Photon Science Group)
PSP	Proposal Study Panel
Q-STXM	STXM endstation optimized for high-field, low-temperature magnetic microscopy
QERLIN	Q- and Energy-ResOLved INelastic Scattering Beamline
QIS	quantum information science
qRIXS	momentum-resolved resonant inelastic x-ray scattering
R&D	research and development
RADSI	relative-angle determinable stitching interferometry
REXS	resonant elastic x-ray scattering
rf	radiofrequency
RIXS	resonant inelastic x-ray scattering
rms	root-mean-square
RSoXS	resonant soft x-ray scattering
RSS	radiation safety system
s-SNOM	scattering type, scanning near-field optical microscopy
SAC	Scientific Advisory Committee
SAXS	small-angle x-ray scattering
SIBYLS	Structurally Integrated BiologY for the Life Sciences
SINS	synchrotron infrared nanospectroscopy
SLAC	SLAC National Accelerator Laboratory
STTR	Small-Business Technology Transfer
STXM	scanning transmission x-ray microscopy
SXR	soft x-ray
TA	Thrust Area
TBD	to be determined
TReXS	tender resonant x-ray scattering
UC	University of California
UEC	Users' Executive Committee
UHV	ultrahigh vacuum
USGS	United States Geological Survey
VUV	vacuum ultraviolet
WAXS	wide-angle x-ray scattering
XAS	x-ray absorption spectroscopy
XFEL	European X-Ray Free-Electron Laser Facility
XMCD	x-ray magnetic circular dichroism
XMLD	x-ray magnetic linear dichroism

XPCS	x-ray photon correlation spectroscopy
XPS	x-ray photoelectron spectroscopy
XRD	x-ray diffraction
XRF	x-ray fluorescence
XROL	X-Ray Optics Laboratory